



BOOK OF ABSTRACTS

30 AUGUST–3 SEPTEMBER 2026

21st International Conference on Defects Recognition,
Imaging and Physics in Semiconductors

SCIENTIFIC PROGRAMME • ORAL & POSTER ABSTRACTS

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01

Oxides

MONDAY · 31 AUGUST 2026

08:50–10:30

Hall of Mirrors

Chair: Julita Smalc-Koziorowska

PRESENTATIONS

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Effects of Oxygen Vacancies on Time-Dependent Dielectric Breakdown in Hafnia Ferroelectrics

The wide variety of vacancy defects in β -Ga₂O₃

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Theoretical calculations [1, 2] of defect properties in β -Ga₂O₃ predict unusually low formation energies for Ga vacancy related defects in all of their negative charge state configurations at Fermi levels near the conduction band edge. Hence Ga vacancy defects should be abundant and efficiently compensate for *n*-type doping. Even complexes involving a Ga vacancy, O vacancy, and two hydrogen atoms are predicted to exhibit negative charge states at high Fermi levels. There is also abundant experimental evidence obtained by IR spectroscopy, EPR spectroscopy, positron annihilation spectroscopy and transmission electron microscopy that (split) Ga vacancies are present at very high concentrations in β -Ga₂O₃ irrespective of doping or conductivity [3]. Theory also predicts that these split Ga vacancies have the lowest formation energies. Many different split Ga vacancy configurations are predicted to form. Why these defects are not efficient in compensation of the donors, leading to easily controllable *n*-type doping, remains an open question.

We have performed temperature and orientation dependent positron annihilation experiments in a wide variety of *n*-type and semi-insulating β -Ga₂O₃ and β -(Al,Ga)₂O₃ single crystals and thin films [4]. The colossal anisotropy of the positron annihilation signals allows to identify certain types of defects that dominate the experimental data [5]. We show that split Ga vacancies in various configurations are the main defect observed with positron annihilation in almost all as-grown β -Ga₂O₃ samples. Unrelaxed Ga vacancies can be introduced by high-energy particle irradiation at room temperature, and they relax to the split configuration upon thermal annealing [6, 7]. Employing Si as an *n*-type dopant promotes the formation of unrelaxed Ga vacancies in particular in the β -(Al,Ga)₂O₃ alloys [7]. In spite of the high concentrations of the Ga vacancy related defects in the as-grown materials, the electrical compensation appears not to be directly affected by the vacancies.

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Formation and stabilization of Ga vacancies in β -(Al,Ga) $_2$ O $_3$: effects of Al-alloying, Si-doping, and proton irradiation

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While *n*-type doping is readily achieved in β -Ga $_2$ O $_3$, its realization in wider band-gap β -(Al,Ga) $_2$ O $_3$ alloys remains challenging due to compensating defects. Here, we investigate cation vacancy formation in Si-doped β -(Al,Ga) $_2$ O $_3$ single crystals using positron annihilation spectroscopy. Eight Czochralski-grown crystal samples with Al contents of 0-25% were studied in both undoped and Si-doped forms. The investigated crystals were grown at Leibniz-Institut für Kristallzüchtung [1]. Residual Si concentrations in nominally undoped samples are $2\text{--}3 \times 10^{17} \text{ cm}^{-3}$, while intentional doping yields $3\text{--}6 \times 10^{18} \text{ cm}^{-3}$. Hall measurements show *n*-type conductivity in undoped samples across all compositions, whereas doping efficiency decreases with increasing Al content and the 25% alloy becomes electrically insulating [1].

Temperature-dependent positron lifetime and 4D Doppler broadening measurements [2] reveal pronounced differences between undoped and Si-doped materials. Undoped crystals exhibit the strong anisotropy characteristic of β -Ga $_2$ O $_3$ [3], while Si-doped samples show strongly reduced anisotropy independent of Al content. Positron lifetimes are longer in Si-doped samples (190–220 ps) than in undoped ones (170–195 ps), indicating enhanced vacancy trapping. The lifetime values for undoped samples are similar to those obtained in Sn-, Fe-, and Mg-doped β -Ga $_2$ O $_3$ crystals [2]. Si-doped alloys with 10–25% Al display nearly identical annihilation characteristics, consistent with dominant unrelaxed Ga vacancies regardless of composition. Undoped samples instead show signatures of split Ga-vacancy configurations, with unrelaxed vacancies appearing only at elevated temperatures for higher Al contents (20–25%). Below 100 K, negatively charged ion-type defects are observed exclusively in Al-containing samples. The nearly identical annihilation signatures of all Si-doped alloys indicate that the insulating behavior of the 25% Al sample cannot be explained by Ga vacancies alone, but likely involves additional acceptor-type defects.

To further probe defect formation, representative samples with the most distinct annihilation characteristics were selected for 6-MeV proton irradiation. Undoped samples (10 and 25% Al) show increased positron lifetimes, reduced Doppler anisotropy, and decreased W_2 parameters, consistent with irradiation-induced formation of unrelaxed Ga vacancies. In contrast, only minor changes occur in Si-doped samples (0 and 25% Al), indicating that such vacancies are already dominant prior to irradiation.

Overall, Al-alloying, Si-doping, and proton irradiation stabilize unrelaxed Ga vacancies and promote negatively charged compensating defects, which limit doping efficiency and contribute to insulating behavior in highly alloyed β -(Al,Ga) $_2$ O $_3$.

Crystal growth was funded by the German Research Foundation (DFG) project no. 491040331.

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Electron microscopy investigation of laterally overgrown α -Ga₂O₃

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The rhombohedral phase of gallium oxide (α -Ga₂O₃) is rapidly gaining attention owing to its potential for bandgap engineering with other rhombohedral sesquioxides and favourable properties for high power device applications.[1] However, it can currently only be grown using heteroepitaxy, primarily on sapphire substrates, resulting in defect generation which would hinder device performance. Epitaxial lateral overgrowth (ELOG) has been developed for α -Ga₂O₃ by partially masking the substrate to promote lateral growth. While ELOG reduces the dislocation density from 10¹⁰ to 10⁷ cm⁻², the effects on other sample properties are still poorly understood.[2,3]

We employed multi-mode microscopy, correlating the optical, chemical and topographic properties of α -Ga₂O₃ ELOG samples in cross-section, employing temperature-dependent cathodoluminescence (CL), energy dispersive X-ray spectroscopy (EDX), and secondary electron imaging. The samples were grown by halide vapour phase epitaxy: a low temperature rapid growth sample involving 520°C growth followed by 486°C growth, and a reference sample grown entirely at 520°C.[4]

Our data shows low temperature growth suppresses point defect formation and promotes dislocation annihilation. CL reveals columnar regions of varying intensity linked to the mask/window ELOG structure, with the window region being 2× brighter than the masked region, contrary to the usual expectation of a less defective mask region. EDX highlights areas of structural imperfection and high dislocation density. We attribute this reduction of luminescence to incorporation of point defects acting as non-radiative recombination centres on the lateral growth facets.

In conclusion, multi-mode microscopy provides a deeper understanding of defect incorporation, highlighting the fundamental impact of growth temperature on the ELOG process and how it can produce higher quality samples, which is essential for informing future growth strategies and paving the way for material that would be more suitable for usage in high power devices.

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Acknowledgments

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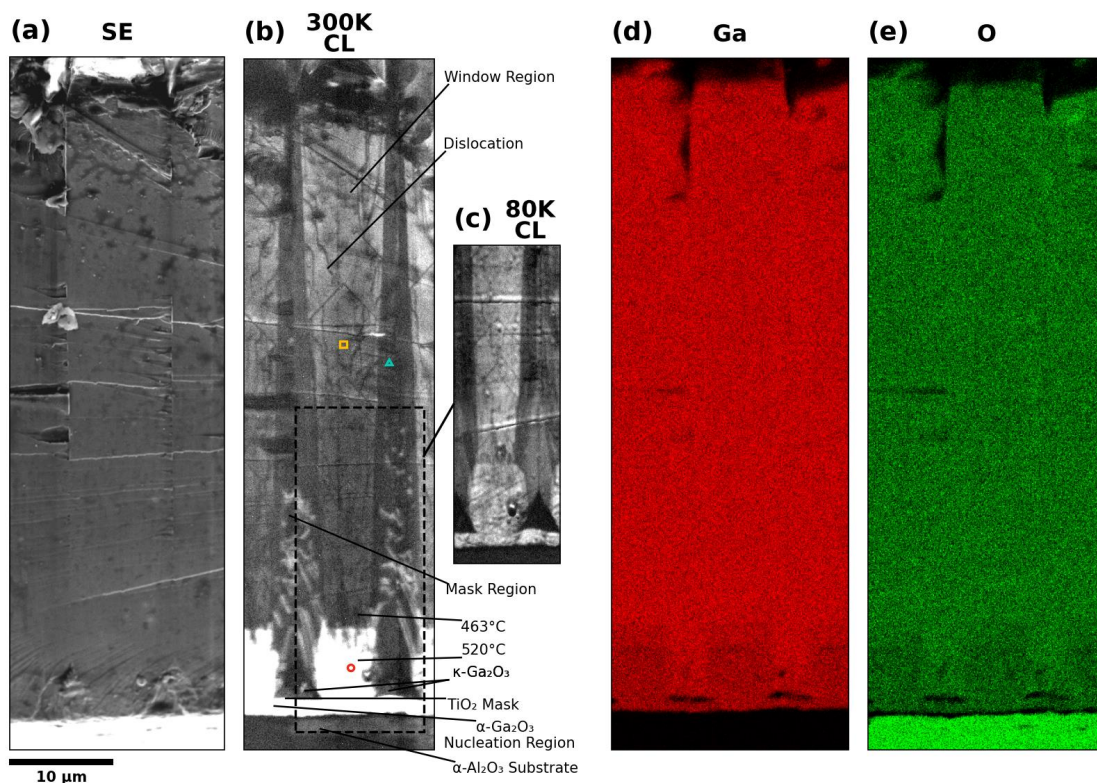


Figure 1: Multi-modal analysis of the low temperature sample observed in cross-section consisting of (a) SE, (b) 300 K CL, (c) 80 K CL, EDX of Ga (d), and O (e)

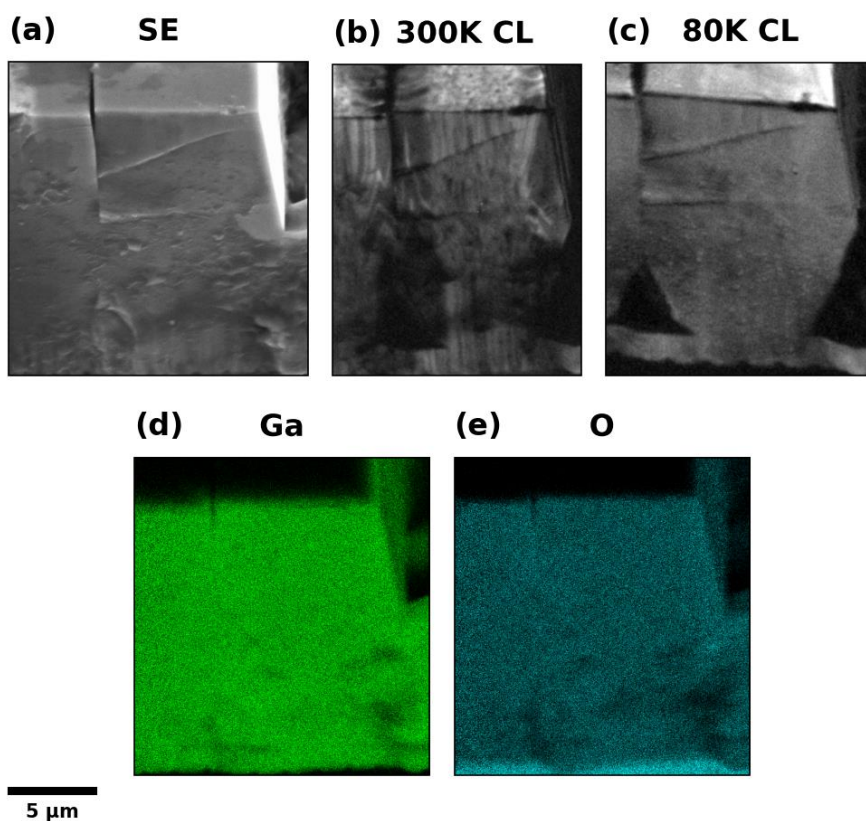


Figure 2: Multi-modal analysis of the reference sample observed in cross-section consisting of (a) SE, (b) 300 K CL, (c) 80 K CL, EDX of Ga (d), and O (e)

Effects of Oxygen Vacancies on Time-Dependent Dielectric Breakdown in Hafnia Ferroelectrics

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Hafnia-based ferroelectrics have attracted significant attention as key materials for next-generation nonvolatile electronic devices owing to their CMOS compatibility and VLSI scalability [1]. In particular, hafnia-based ferroelectric tunnel junctions (FTJs) are promising for low-power memory and neuromorphic applications because their resistance state can be modulated by polarization switching into an ultrathin ferroelectric barrier. Despite this potential, reliability remains a critical issue for practical implementation. Among various defect-related factors, oxygen vacancies are especially important because they strongly affect ferroelectric phase stability, charge transport, leakage behavior, and dielectric degradation [3]. However, their role in time-dependent dielectric breakdown has not been fully clarified, especially in hafnia-based FTJs.

In this study, we investigate the effect of oxygen vacancies on time-dependent dielectric breakdown (TDDB) in hafnia ferroelectric tunnel junctions. Two junction types are compared: an oxygen-vacancy-rich hybrid tunnel junction (HTJ) and an oxygen-vacancy-poor FTJ. Constant-voltage stress measurements were used to monitor leakage-current evolution and identify breakdown events, including current drift, first and second soft breakdown, and hard breakdown. We demonstrate a counterintuitive trend: the oxygen-vacancy-rich HTJ exhibits better TDDB reliability than the oxygen-vacancy-poor FTJ. In the vacancy-poor FTJ, leakage current increases more abruptly and hard breakdown occurs after successive soft-breakdown events. In contrast, the vacancy-rich HTJ shows a more gradual current evolution, delayed hard breakdown, and improved endurance under electrical stress (Fig. 1(a) and (b)). These results indicate that a higher oxygen-vacancy concentration does not necessarily degrade the film; instead, an optimized vacancy population can improve the robustness of hafnia ferroelectric tunnel junctions. The Weibull plots quantify the statistical distribution of t_{DB} for the FTJ and HTJ. Compared with the FTJ, the HTJ shows a pronounced shift to longer t_{DB} and a much larger characteristic lifetime for all device areas. After area normalization the HTJ still exhibits longer t_{DB} than the FTJ, confirming that the improved TDDB reliability is not simply caused by device-area differences but is associated with the oxygen-vacancy-rich ferroelectric layer (Fig. 1(g)). In the vacancy-rich HTJ, pre-existing oxygen vacancies are more uniformly distributed and can partially relax local electric-field concentration and defect-generation stress. Therefore, breakdown proceeds more gradually rather than through rapid localized percolation. The results suggest that controlling oxygen-vacancy concentration is not only important for ferroelectric switching, but also for long-term dielectric reliability.

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Acknowledgment

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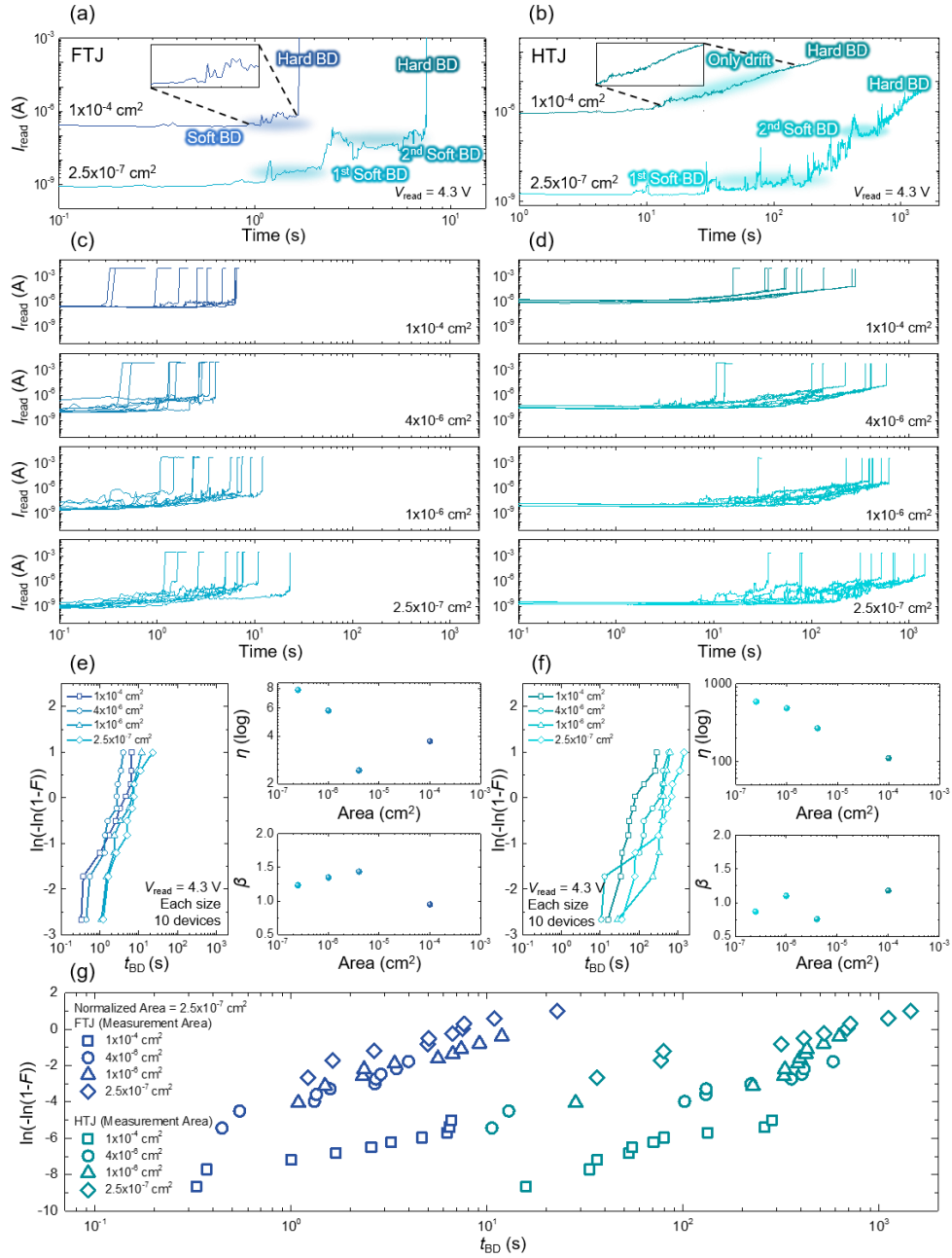


Figure 1. TDDB characteristics of oxygen-vacancy-poor FTJ and oxygen-vacancy-rich HTJ. Representative current transients under constant-voltage stress for (a) FTJ and (b) HTJ, including current drift, soft breakdown, and hard breakdown. Area-dependent TDDB characteristics of (c) FTJ and (d) HTJ measured from devices with different sizes. Weibull plots of breakdown time for (e) FTJ and (f) HTJ, showing a longer characteristic breakdown lifetime in the HTJ. (g) Area-normalized Weibull plot of FTJ and HTJ, confirming that the improved TDDB reliability of the HTJ originates from the oxygen-vacancy-rich ferroelectric layer rather than device-size effects.

02

SiC I

MONDAY · 31 AUGUST 2026

11:00–13:00

Hall of Mirrors

Chair: Balaji Raghothamachar

PRESENTATIONS

- 2.0** **Rong Wang** INVITED
Growth of ultra-thick 4H-SiC single crystal boules and epitaxial films
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Revisiting ECCI as a Technique for Defect Assessment in 3C-SiC

Growth of ultra-thick 4H-SiC single crystal boules and epitaxial films

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4H silicon carbide(4H-SiC) is the material of choice for high-power and high-frequency electronics. In this work, we will introduce the research progress in growing 100-mm grade 4H-SiC single-crystal boules and 300- μ m grade homoepitaxial films.

In order to reduce the cost of 4H-SiC single-crystal substrates, a novel crystal growth method, termed as the pulling physical vapor transport (PPVT) method is proposed to combine the temperature-control and pulling-control strategies^[1]. By in-situ controlling the axial and radial temperature gradients during long-term single-crystal growth, the thermal stress inside 4H-SiC single-crystal boules can be significantly reduced. The PPVT growth experiments were performed to grow 6- and 8-inch 4H-SiC single-crystal boules, achieving crack-free crystals with thickness up to 100 mm and 50 mm, respectively. The significant increase in thickness of 4H-SiC boules would increase the number of substrates produced in each furnace, and hold great promise in reducing the cost of 4H-SiC substrates [Fig. 1].

During homoepitaxy, 4H-SiC epitaxial films with thickness of 312 μ m has been developed addressing the demand of ultra-high power devices including smart grids, offshore wind powers and radiation detectors. We reveals the effect of growth rate and C/Si ratio on the step-flow growth and the surface morphology of 4H-SiC epitaxial layers, establishing the desired process window for the rapid epitaxy of 4H-SiC ultra-thick epitaxial layers. With the growth rate as high as 120 μ m/h, the ultra-thick 4H-SiC epitaxial layer with the thickness of 312 μ m is prepared, with the surface morphological defect density being 0.75 /cm². This indicates favorable defect control capability during the fast epitaxy process. The average minority carrier lifetime of the 310- μ m 4H-SiC ultra-thick epitaxial layer is 741 ns, which is affected by basal plane dislocations (BPDs) induced by the internal stress [Fig. 2]^[2].

As BPDs can't be eliminated from 4H-SiC epitaxial films, a non-thermodynamic equilibrium post-treatment method is proposed to suppress the bipolar degradation in 4H-SiC devices by promoting shrinkage and even elimination single Shockley stacking faults (1SSFs). We propose a combined approach of low-power UV irradiation and thermal annealing to promote the extraction of electrons from the defect levels of 1SSFs, thus promote the shrinkage and even elimination of 1SSFs [Fig. 3]^[3].

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Acknowledgment

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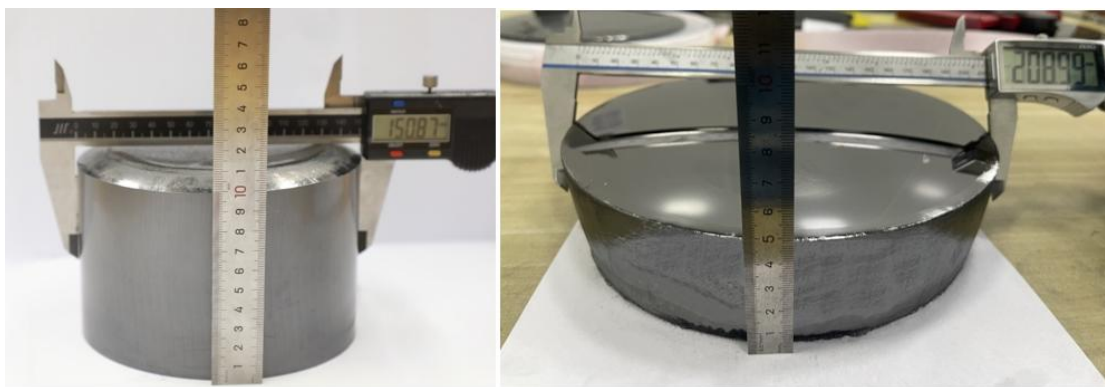


Figure 1: Crack-free 6- and 8- inch 4H-SiC single-crystal boules grown by the PPVT method.

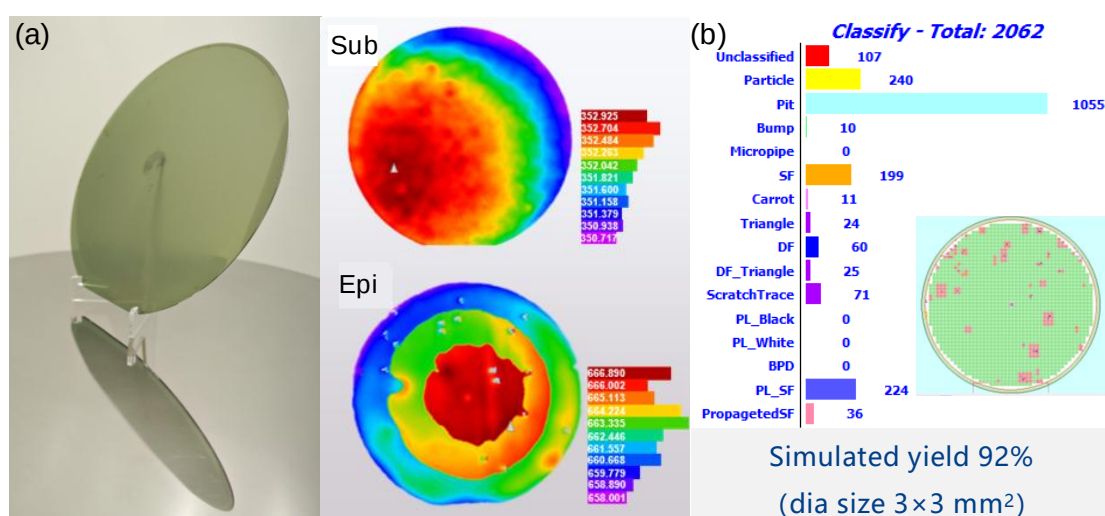


Figure 2: (a) Photograph and change of thickness before and after epitaxy of ultra-thick 4H-SiC films. (b) Distribution of defects and simulated yield of the 312- μ m 4H-SiC film.

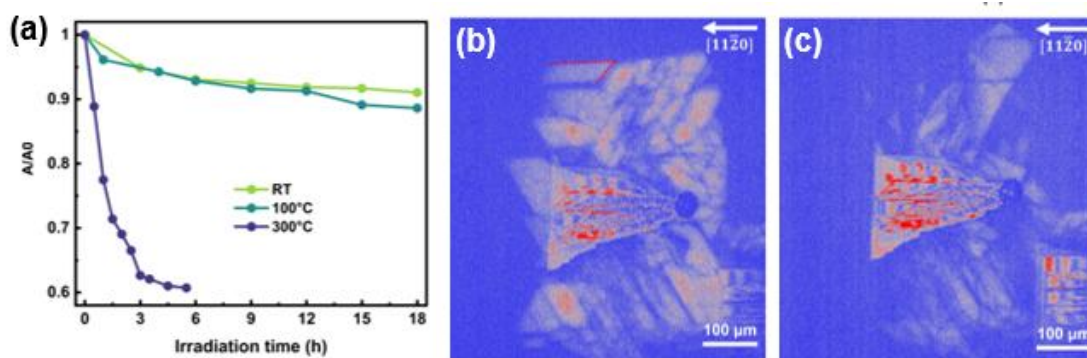


Figure 3: (a) Relative change of the total area of 1SSFs under low-power UV illumination at different temperatures. A_0 and A are the initial and remaining total areas of 1SSFs before and after low-power UV illumination. PL images illustrating 1SSFs surrounding the comet defect (b) before and (c) after the synergistic low-power UV irradiation and thermal treatment at 300 °C.

Deep-Level Traps in 4H-SiC Bulk Single Crystals Grown by High-Temperature Chemical Vapor Deposition

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Generally, 4H-SiC bulk single crystals are currently produced by the sublimation (physical vapor transport) method, which remains the industrial mainstream for substrate supply. In contrast to the extensive literature on deep-level traps in 4H-SiC epitaxial films, studies directly targeting traps in bulk crystals by deep-level transient spectroscopy (DLTS) have been relatively limited in practice. One practical reason is that bulk substrates are often either low-resistivity (highly doped n^+ -type) or semi-insulating, which can impose constraints on forming a well-behaved depletion region and acquiring high signal-to-noise capacitance transients in junction-based DLTS measurements. Recently, high-temperature chemical vapor deposition (HTCVD), which is performed at 2500–2550 °C using SiH_4 and C_3H_8 as source gasses, is attracting attention as a fast bulk-growth approach capable of high growth rates and improved crystal quality [1]. In particular, growth rates on the order of $\sim 3 \text{ mm h}^{-1}$ and significant reductions of dislocation densities along the growth direction have been demonstrated [2], motivating systematic defect spectroscopy for HTCVD-grown bulk crystals.

Here, we investigated deep-level traps in an HTCVD-grown 4H-SiC bulk crystal by DLTS, complemented by secondary ion mass spectrometry (SIMS). To enable DLTS measurements on a bulk crystal, we prepared an n^-/n^+ structure by growing a nominally n -type, lightly N -doped (n^-) 4H-SiC layer by HTCVD on a highly N -doped n^+ seed crystal, and then cutting out specimens for Schottky diode fabrication and electrical characterization (Figure 1). SIMS indicated representative unintentional impurities of N on the order of 10^{16} cm^{-3} and B on the order of 10^{15} cm^{-3} in the HTCVD-grown bulk samples.

The DLTS measurements revealed multiple traps, including a dominant peak near $\sim 280 \text{ K}$ (Figure 2). Compared with an electron-irradiated n^- epitaxial film reference used as a carbon-vacancy-related $Z_{1/2}$ marker, the dominant peak in the HTCVD-grown sample was slightly shifted to lower temperature. Electric-field dependence measurements further suggested donor-like, field-enhanced emission behavior for the dominant HTCVD peak, whereas the $Z_{1/2}$ marker peak showed weak field dependence. After electron irradiation of the HTCVD-grown crystal, the dominant peak intensity increased and the peak position became intermediate between the as-grown HTCVD peak and the $Z_{1/2}$ marker peak, suggesting a superposition of at least two defect contributions: an HTCVD-intrinsic component and an irradiation-induced component. Overall, the peak shift, field response, and marker-assisted intermediate peak position indicated that the dominant HTCVD peak is not solely attributable to $Z_{1/2}$ and likely includes an intrinsic donor-like contribution, although definitive identification requires additional constraints.

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Acknowledgment

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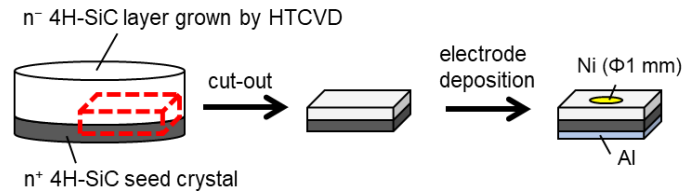


Figure 1: Schematic of DLTS sample preparation. An n^- 4H-SiC layer grown by HTCVD on an n^+ 4H-SiC seed crystal was cut out and processed into a Schottky diode by depositing a circular Ni contact ($\Phi 1\text{ mm}$) on the top surface and an Al back contact.

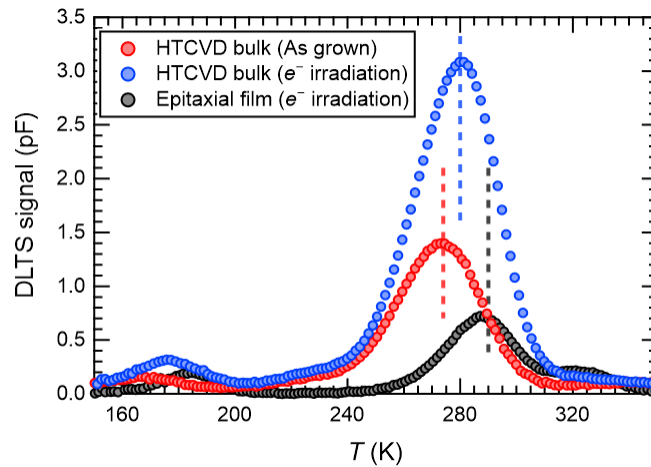


Figure 2: DLTS spectra of an HTCVD-grown 4H-SiC bulk crystal (as-grown, red), the same HTCVD crystal after electron irradiation (blue), and an electron-irradiated reference epitaxial film as $Z_{1/2}$ marker (black). Measurement conditions: reverse bias $V_R = -10\text{ V}$, pulse bias $V_P = 0$, pulse width $t_p = 5\text{ ms}$, and rate window $T_W = 409.6\text{ ms}$.

Electronic properties of silicon vacancies in semi-insulating 4H-SiC

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The negatively charged silicon vacancies ($V_{\text{Si}}(-)$) are point defects in the silicon carbide (SiC) crystal lattice playing the role of artificial atoms whose internal spin-optical transitions can be used in technology of various quantum devices for specific applications in the areas of quantum sensing, communication, and computing [1]. The 4H-SiC polytype is predominantly used for quantum applications due to its wide bandgap (3.36 eV at RT) and high crystalline quality. According to the structure of 4H-SiC lattice, there are two inequivalent lattice sites to be occupied by V_{Si} , namely hexagonal (h) and quasi-cubic (k) sites. The $V_{\text{Si}}(-)$ located at each site has five electrons, including those originating from the four sp^3 dangling bonds surrounding the defect and an additional captured from the conduction band. The $V_{\text{Si}}^h(-)$ and $V_{\text{Si}}^k(-)$ are identified by the zero-phonon lines (ZPLs) which are best resolved in the near-infrared region of the photoluminescence (PL) spectrum measured at cryogenic temperatures. The former gives rise to the V1 and V1' ZPLs centered at 1.438 eV (~861.8 nm) and 1.443 eV (~859.3 nm), respectively [1]. The latter generates the V2 ZPL at 1.352 eV (~917.6 nm) [1]. So far, however, the energy levels of the (0/-) charge state transitions for the V_{Si}^h and V_{Si}^k have not been determined experimentally. On the other hand, the calculations based on the usage of the Hyde-Scuseria-Ernzerhof (HSE06) hybrid functional have indicated that the charge state transition levels for the $V_{\text{Si}}^h(0/-)$ and $V_{\text{Si}}^k(0/-)$ are located at the energies of 1.28 and 1.25 eV above the valence band maximum (VBM), respectively [2].

In this paper, for the first time we demonstrate the experimental energy values for the $V_{\text{Si}}^h(0/-)$ and $V_{\text{Si}}^k(0/-)$ transitions. The results were obtained by the High-Resolution Photoinduced Transient Spectroscopy (HRPITS) measurements using the samples of high-purity semi-insulating (HPSI) 4H-SiC subjected to rapid thermal annealing (RTA) at 700 °C for 3 min in N₂ atmosphere. The Fermi-level position in the material, determined from the dark current temperature dependence in the range of 500 – 750 K, was at the energy of 1.32 eV with respect to the energy of the VBM. The high material resistivity of the order of 10⁹ Ωcm at RT was due to the compensation of the shallow donors, formed by the residual nitrogen atoms, by the deep acceptors, formed by the negatively charged silicon vacancies. The charge state transitions $V_{\text{Si}}^h(0/-)$ and $V_{\text{Si}}^k(0/-)$, were resolved in the photocurrent relaxation waveforms induced by the thermal emission of holes occurring after switching off the UV excitation pulse generating the excess electrons and holes. The waveforms, recorded at temperatures 500 – 750 K, were transformed into the two-dimensional (2D) correlation and Laplace spectra, allowing for determining the temperature dependences of the thermal emission rate of holes related to the $V_{\text{Si}}^h(0/-)$ and $V_{\text{Si}}^k(0/-)$ transitions. Figure 1(a) shows the 1D correlation spectra, obtained by the cross-sections of the spectral surface at the specific emission rates, and Figure 1(b) illustrates the Arrhenius plots for the thermal activation of the emission holes as well as the values of the activation energy E_a and the values of the pre-exponential factor A in the Arrhenius equation. These results are of great importance for identification of quantum defects in 4H-SiC.

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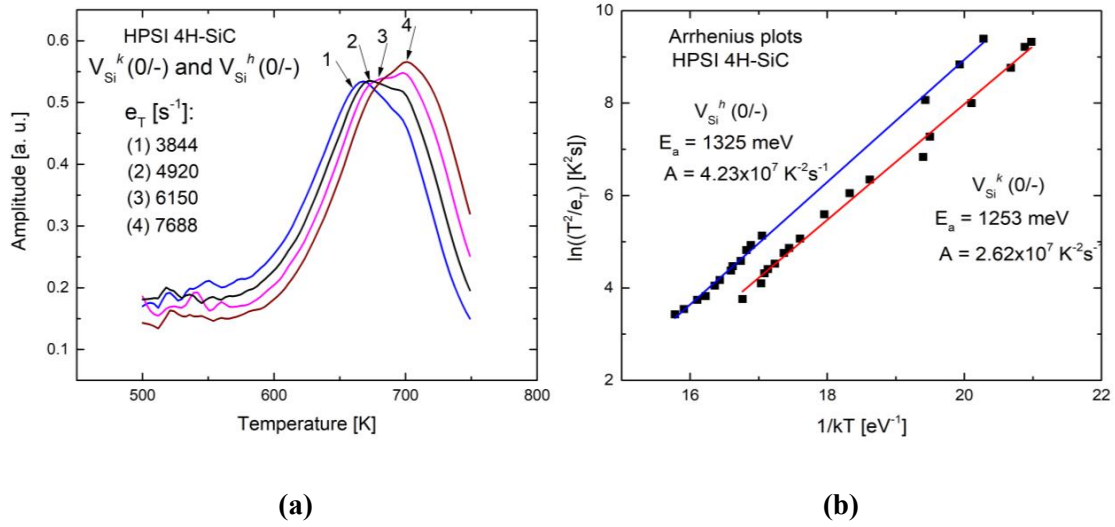


Figure 1: (a) One-dimensional correlation spectra resolved by HRPITS for the four values of the thermal emission rate of holes from silicon vacancies in HPSI 4H-SiC. The maxima indicate the temperatures corresponding to the emission rates values for the specific charge state transitions. (b) The Arrhenius plots for the thermal activation of holes leading to the (0/-) charge state changes of the silicon vacancies located in the h and k sites of the 4H-SiC crystal lattice. The solid lines are fitted by linear regression to the experimental data. The E_a and A values are obtained from the slope and intercept of these lines, respectively.

Electron Transport and Dislocations in Heavily Doped and Co-Doped n-Type 4H-SiC

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The development of low-resistivity substrates is crucial for advancing high-power and high-frequency devices based on 4H-SiC. In this work, heavily doped 4H-SiC single crystals, including nitrogen-doped, nitrogen–aluminum (N–Al) co-doped, and nitrogen–gallium (N–Ga) co-doped samples, were grown using the physical vapor transport (PVT) method.

A comparative investigation was conducted to evaluate the effects of co-doping on nitrogen incorporation, electrical transport properties, and crystal defects. The results demonstrate that both N–Al and N–Ga co-doping significantly enhance nitrogen incorporation efficiency, leading to a marked reduction in resistivity compared to single nitrogen doping. Furthermore, heavy doping is found to shift the Fermi level into the conduction band, indicating a transition toward degenerate semiconductor behavior.

Temperature-dependent mobility measurements reveal that electron transport exhibits thermally activated behavior above 300 K, suggesting the involvement of impurity-related scattering mechanisms. In terms of crystal quality, the incorporation of Al and Ga atoms effectively suppresses the glide and multiplication of basal plane dislocations (BPDs), resulting in a reduced BPD density. Notably, N–Ga co-doping shows a pronounced effect in suppressing the formation of stacking faults, as shown in Figure 1.

These findings highlight the effectiveness of co-doping strategies in simultaneously improving electrical conductivity and crystalline quality of 4H-SiC, providing a promising pathway for the fabrication of low-resistivity SiC substrates for advanced electronic applications.

Acknowledgment

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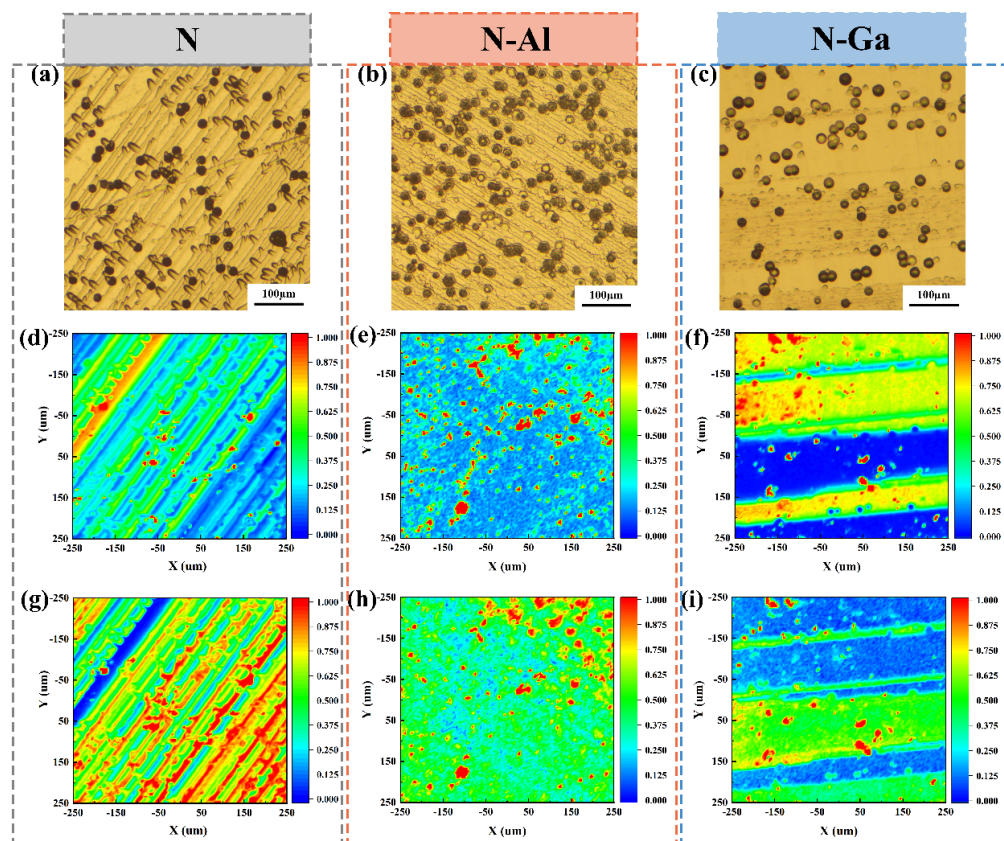


Figure 1. (a)-(c) The optical microscopy images, (d)-(f) photoluminescence (PL) intensity mapping at the wavelength of 393 nm, and (g)-(i) PL intensity mapping at the wavelength of 500 nm for the heavily N-doped, N-Al co-doped, and N-Ga co-doped 4H-SiC.

Revisiting ECCI as a Technique for Defect Assessment in 3C-SiC

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Electron contrast channeling imaging (ECCI) is a scanning electron microscope (SEM) based technique that can directly image strains, and thus crystalline defects, within the near surface across whole individual crystals. It is similar to two-beam transmission electron microscopy (TEM) diffraction, it is achieved by exploiting the orientation sensitive channeling of backscatter electrons when the crystal is orientated at/close to the Bragg condition (fig. 1c) [1], [2]. Despite being developed decades ago, ECCI, has recently gained interest and popularity over time with advances in SEM and backscatter detector technology [2], [3]. One point of resurgence in the 2000's on semiconductor materials had the stage tilted at a high angle in electron backscatter diffraction (EBSD) conditions and used its forescatter detectors to achieve ECCI (fig. 1a).

3C-SiC has increasingly become an attractive semiconductor in the fields power electronics, quantum, etc. [4], with recent research into reducing the defect density in 3C-SiC such as switchback epitaxy [5] and trench epitaxy [6]. Typical methods of defect detection such as PL, XRT or selective defect etching are not suitable or appropriate for 3C-SiC technology due to the level and type of defects which are typically stacking faults, microtwins and threading dislocations, as well as the use of Si as the substrate [6]. ECCI, then provides an attractive alternative to TEM methods to assess these defects, especially as an alternative to plan-view TEM. However, to the authors knowledge, the last known published cases of ECCI for 3C-SiC defect assessment were three papers in the late 2000's using the forescatter setup [7], [8], [9].

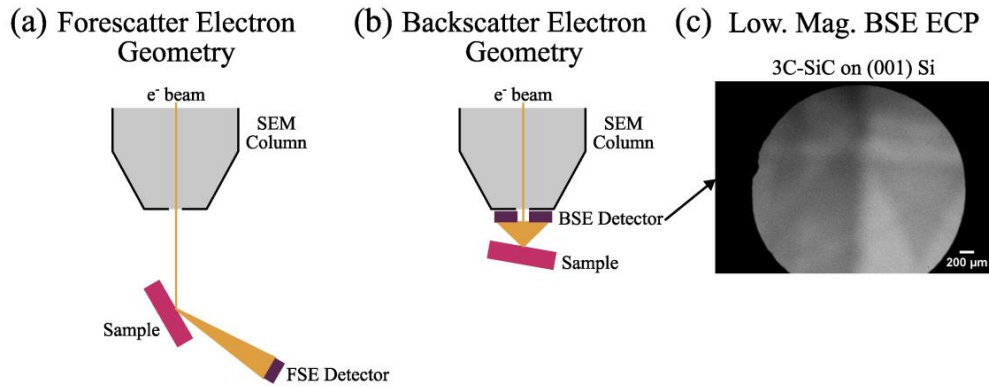
In this work, the authors revisit performing ECCI on 3C-SiC, but now exploiting the backscatter ECCI geometry (fig. 1b), which has increased in popularity partly due to the technological and methodology improvements [2] and its greater defect contrast and spatial resolutions [1]. The aims are to show that ECCI can be standardized and is a promising method to assess the extended defect density in epitaxial 3C-SiC (fig. 2). To show this the defect densities of samples of increasing thicknesses will have their ECCI defect densities compared with those from cross-sectional TEM results, which will act to validate the technique as it is known that increasing the epitaxial 3C-SiC thickness decreases the defect density [6].

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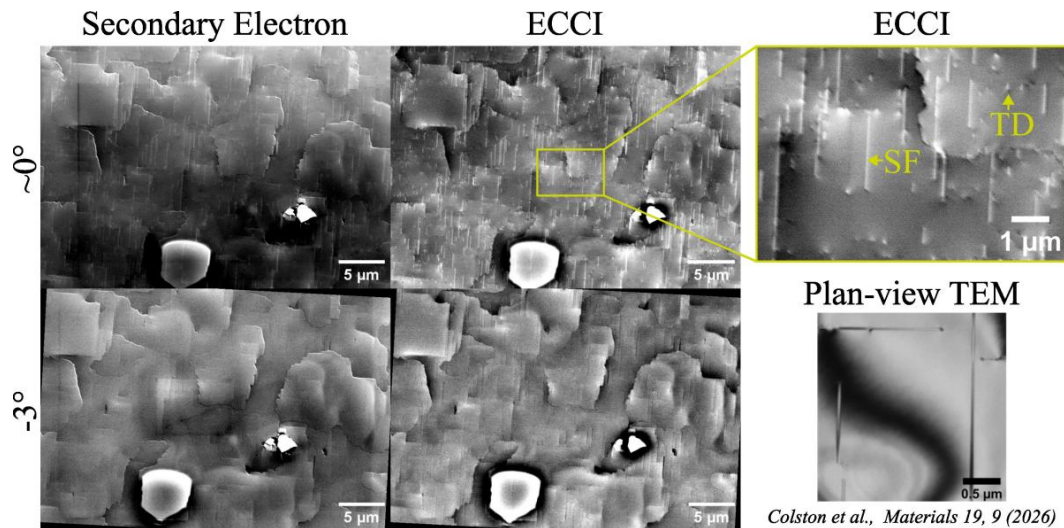
Acknowledgment

We acknowledge the EPSRC grant EP/W004291/1, InnovateUK grant 10110043, EPSRC grant UKRI637, and the David Cockayne Centre for Electron Microscopy, Department of Materials, University of Oxford.



Adapted from S. Zaefferer et al., *Acta Materialia*, 75, 20–50, (2014)

Figure 1: Schematic geometries of the (a) forescatter and (b) backscatter ECCI setups, adapted from [1]. (c) is a low magnification BSE signal electron channeling pattern (ECP) collected from epitaxial 3C-SiC on (001)-surface silicon substrate under the $g=\{2\ -2\ 0\}$ diffraction condition.



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Figure 2: Brightness and contrast enhanced secondary electron and backscatter electron (i.e. ECCI) signals of the sample in fig. 2c under high magnification under $g=\{2\ -2\ 0\}$. Images at 0° and -3° misorientation away from the diffraction condition in fig. 2c show the decrease in BSE signal contrast from the defects when away from the diffraction condition. The higher magnification ECCI micrograph has arrows pointing to a stacking fault (SF) and a threading dislocation (TD). The plan-view TEM from the same sample [5] shows similar features with ECCI but with over 150 times larger field-of-view.

03

Characterisation

MONDAY · 31 AUGUST 2026

14:30–16:30

Hall of Mirrors

Chair: Jose Coutinho

PRESENTATIONS

- 3.0** **Martien den Hertog** INVITED
Measuring electric properties in semiconducting materials using 4D STEM and electron beam induced current
- 03.1** **Oscar Martínez**
Analysis of asynchronous daylight Electroluminescence and Photoluminescence images of photovoltaic modules under varying irradiance conditions
- 03.2** **Katharina Witzmann**
Inside the crystal: 3D precipitate mapping in semiconductor crystals using optical coherence tomography
- 03.3** **Martin Herms**
Quantitative Stress Evaluation of Semiconductor Wafers by Scanning Infrared Depolarization
- 03.4** **Karolina Fichtova**
Revelios. Semi-automated, non-destructive crystalline defect metrology for GaN based epitaxial layers

Measuring electric properties in semiconducting materials using 4D STEM and electron beam induced current

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Four-dimensional scanning transmission electron microscopy (4D-STEM) is a technique where the electron beam is scanned point by point over the sample, and a diffraction pattern is acquired at each point of the scan, see Fig. 1a. In the presence of an internal electric field, the electron beam is deflected and measuring this deflection allows to probe the material electric properties at high spatial resolution [1–3]. 4D-STEM is developing rapidly, thanks to the development of fast pixelated detectors. The main challenge for quantitative electrical characterization consists in reliably disentangling electrical signal and material contrast from *e.g.* composition/thickness gradients or diffraction contrast. One possibility to facilitate this task is to use in-situ biasing, in order to vary only the electrical part of the signal. Another possibility is to use precession of the electron beam [2]. Moreover, combining 4D-STEM with electron beam induced current (EBIC) can give complementary information on the location and extension of the electric field, without being influenced by diffraction contrast.

In this presentation we will show recent results we obtained using 4D-STEM on a silicon lamella containing a p-n junction. We will show a study on how the quantification, sensitivity and spatial resolution of electric field mapping in a silicon p-n junction are influenced by the acquisition parameters in a momentum resolved 4D-STEM experiment [4–6] analysing the data with the Center of Mass (CoM) approach. It is observed that the electric field precision is improved decreasing the semi-convergence angle, at the cost of decreased spatial resolution. We then combine in-situ electrical biasing and 4D-STEM, allowing to study in more detail the junction abruptness [7], see Fig. 1b,c.

Going beyond lamella samples, we develop a nanosphere based top-down approach to fabricate p-n junction GaN nanowires (NWs) [8,9]. These NWs are then electrically contacted on TEM compatible SiN membranes [10] and studied both electro- optically as UV photo detectors as well as by 4D-STEM and EBIC, allowing better understanding of photo detector performance.

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Acknowledgment

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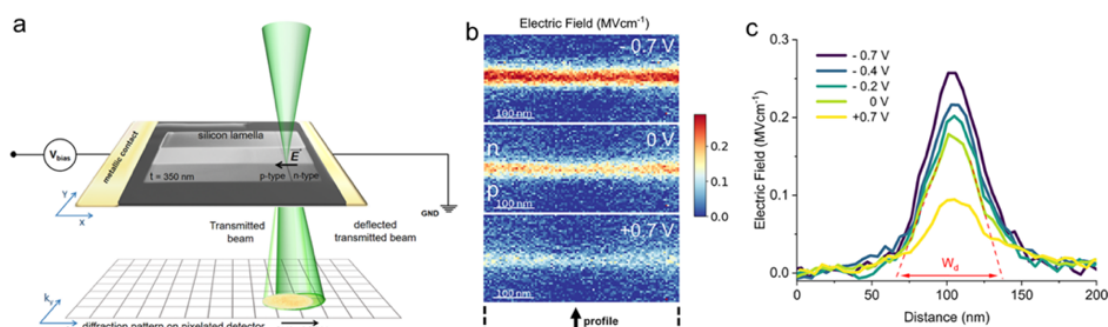


Figure 1a) Schematic of 4D-STEM on a p-n junction. b) Electric field maps on this sample with different values of applied bias. c) Profiles obtained from the maps in a [7].

Analysis of asynchronous daylight Electroluminescence and Photoluminescence images of photovoltaic modules under varying irradiance conditions

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Daylight electroluminescence (dEL) and photoluminescence (dPL) are well-established non-destructive techniques for field inspection of photovoltaic (PV) modules [1,2]. While both methods enable defect detection without controlled laboratory conditions, a systematic quantitative comparison of their imaging performance under varying acquisition conditions remains limited.

This work presents a comparative study of asynchronous [3] dEL and dPL images acquired at multiple irradiance levels (approximately 100–900 W/m²) and adjusted acquisitions parameters (current modulation frequency, camera velocity, exposition time and lens aperture) as needed, evaluating how signal quality and image fidelity evolve with irradiance for each technique. Signal-to-noise ratio (SNR) metrics are computed for each method and irradiance condition to assess how dEL and dPL performance changes across the irradiance range. Additionally, the structural similarity index (SSIM) [4] is applied to directly compare the resultant dEL and dPL images, assessing the degree of perceptual similarity between both luminescence modalities under equivalent acquisition conditions.

Figure 1 compares a dEL and a dPL image at similar irradiance levels using SSIM, providing a color map where values close to 1 indicate perfect similarity, along with a global value representing the overall perceptual resemblance between both images. It is hypothesized that dEL and dPL exhibit distinct SNR vs. irradiance dependencies: for dPL, the relationship is complex, since lower irradiance reduces noise but simultaneously weakens the signal, as photoluminescence relies on irradiance as its excitation source. For dEL, an inverse relationship is expected, where lower irradiance reduces noise and should therefore yield higher SNR values. SSIM analysis will further quantify the perceptual differences between dEL and dPL image outputs, allowing the consistency of the SNR-based comparisons to be validated – with the expectation that images of similar SNR contain comparable perceptual information. These findings will contribute to establishing objective criteria for selecting the most appropriate luminescence technique depending on field conditions, supporting both visual inspection workflows and automated diagnostic algorithms for PV module assessment.

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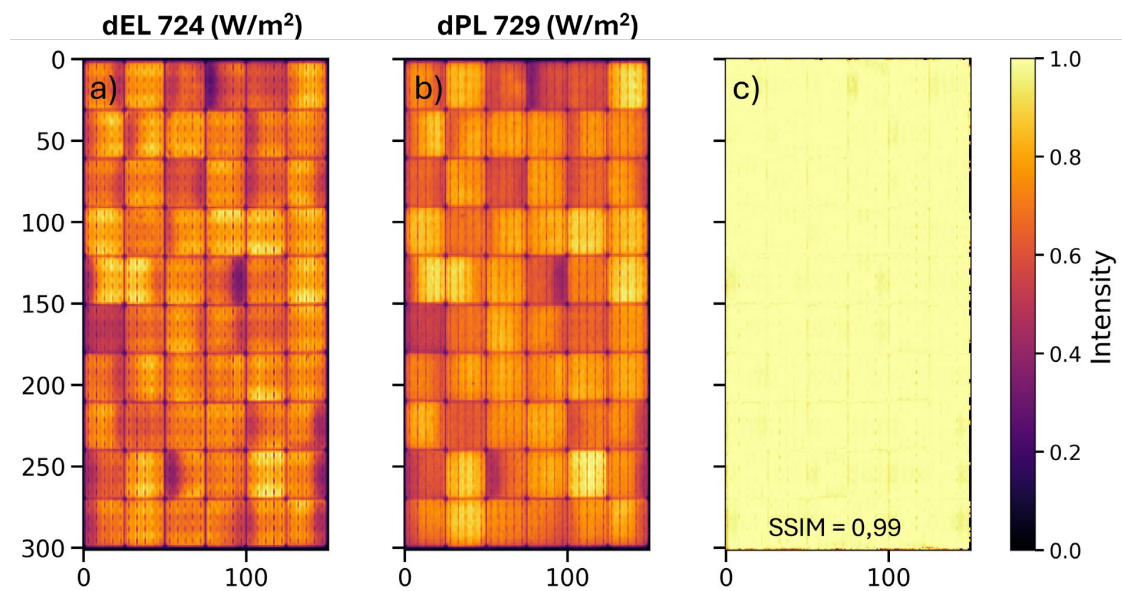


Figure 1: Comparison between dEL and dPL resultant images: a) dEL image, b) dPL image, c) SSIM map comparing image a) vs image b)

**Inside the crystal:
3D precipitate mapping in semiconductor crystals using optical coherence
tomography**

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Dislocations, as extended one-dimensional lattice defects in crystals, have a major impact on their mechanical, electronic, and optical properties. As local disturbances in the periodic atomic arrangement, they influence the movement of charge carriers, recombination in semiconductors, and the strength and deformability of a material. Most experimental methods provide either only two-dimensional projections, surface-near information, or are limited to very small volumes still requiring high preparation effort. This allows the dislocation structure to be reconstructed in sections or sub-areas, but not to trace the complete spatial course of individual dislocations across larger sample dimensions.

Optical coherence tomography (OCT) offers a novel method to obtain three-dimensional information about the dislocation structure. OCT uses near-infrared (NIR) laser light of $\lambda=1,3\mu\text{m}$ to assess the interior of the crystal material. The NIR-beam is reflected by precipitates and inclusions in the material. Based on the operating principle of a Michelson interferometer, the penetration depth of the beam can be varied, providing the Z-location of the precipitates. The precipitates at the dislocations reveal the progression of the decorated dislocations in three dimensions.

In our OCT device, the change in optical path lengths does not occur through the movement of a reference arm, but through the tuning of the wavelength of the short-coherent NIR light with low bandwidth. The backscatter information and sample depth are obtained by Fourier transformation of the phase delay of the reflected light as a function of the wave number. A recording frequency of 100 kHz enables a fast recording of three-dimensional images.

OCT makes it possible to track dislocations in the material and analyze the mechanisms of their formation and decoration. Identifying the relationship between dislocation etch pits and the projection of OCT mapping, as shown in figure 2, offers the possibility of characterizing different types of dislocations. In addition, the behavior of crystal defects such as twin lamellae or polycrystals can be investigated with a new level of accuracy.

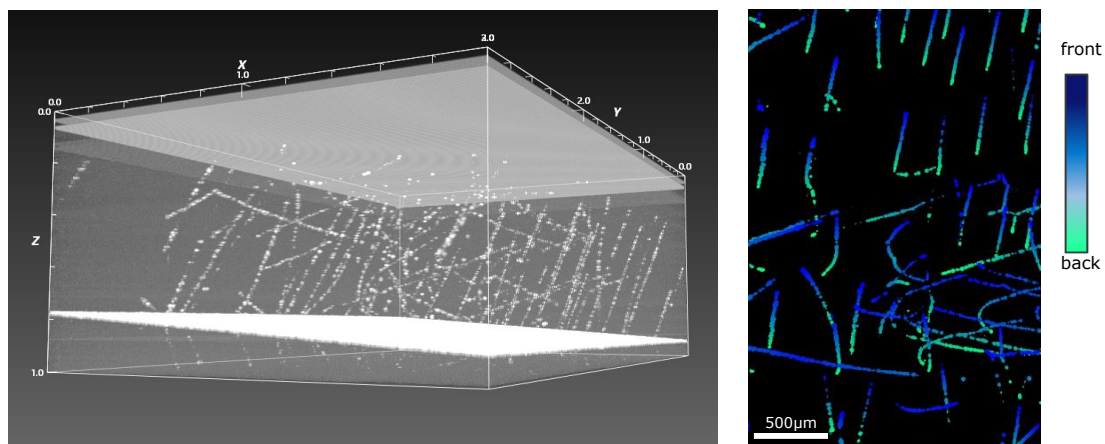


Figure 1: Right: 3D imaging of decorated dislocations using OCT. The signal is generated by the reflection of IR light from precipitates in the material. Left: Color-coded depth-projection of the OCT image onto the wafer surface plane. The color coding delivers the depth information of the precipitates and therefore visualize the progression of the dislocations (facing wafer front – blue, facing wafer back – green).

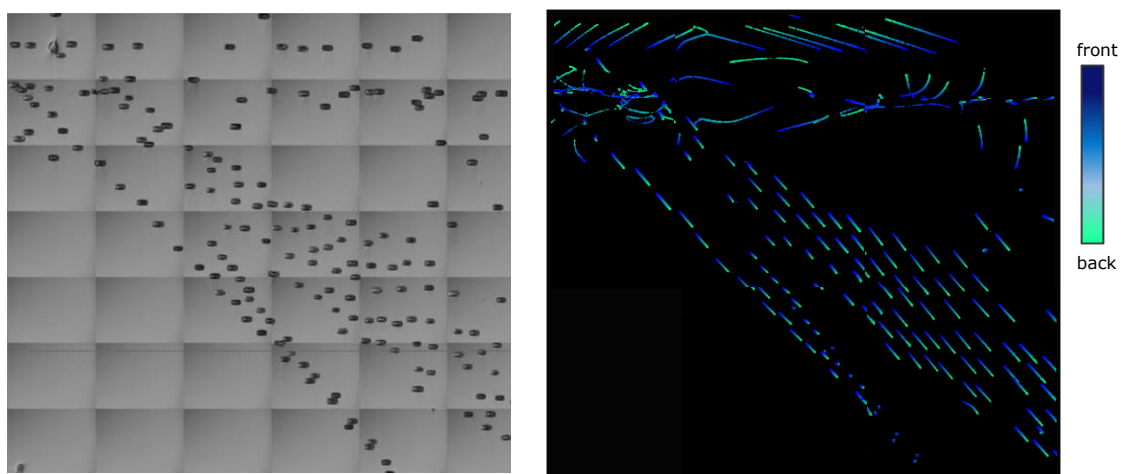


Figure 2: Dislocation Etch pits (left) can be assigned to the depth-projected dislocations lines measured with OCT (right). OCT reveals different types of lattice displacement.

Quantitative Stress Evaluation of Semiconductor Wafers by Scanning Infrared Depolarization

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Scanning Infrared Depolarization (SIRD) is an instrumentation which has been developed and applied for a long time for quality control and process monitoring of Si wafers under industrial conditions [1] with special emphasis on the recognition of defects and the evaluation of residual stress states. The system is continuously tailored for other materials and technologies. Its application to GaAs has also been described in several reports [2] and recently it has been further demonstrated for SiC [3] and AlN [4]. To our knowledge, studies on InP from other groups date back more than 20 years [5, 6].

SIRD exploits the phenomenon of optical birefringence, which is caused by the anisotropy of the refractive index, either natively (intrinsic) or induced by stress. The birefringence changes the polarization of the near-infrared laser beam that scans the sample, which results in a map of depolarization. SIRD systems are presented which work with different scanning modes.

If depolarization is induced by stress, the map can be converted to shear stress by applying the stress-optic law. For this conversion, the photo-elastic constant C_s must be known. C_s varies depending on the material and crystallographic direction. Especially, there has been a lack of experimental data for the case of InP. Hence, C_s was determined for the corresponding crystallographic directions using a special calibration procedure. These values are compared with theoretical and experimental data from the literature for Si, GaAs, InP and SiC, respectively.

The new C_s values were then applied to the stress analysis of wafers made of various materials, as mentioned above, using the multi-polarization analysis, which enables the mapping of the magnitude and direction of residual stress fields.

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Revelios. Semi-automated, non-destructive crystalline defect metrology for GaN based epitaxial layers

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Threading dislocations (TDs) are critical crystalline defects in GaN-based materials, significantly impacting the performance, reliability, and lifetime of electronic and optoelectronic devices. We present Revelios, a semi-automated, non-destructive crystalline defect metrology software prototype based on electron channeling contrast imaging (ECCI). Revelios SW prototype enables large-area acquisition, automated stitching, detection and classification of TDs into a-, c-, and a+c-types. Dislocation type is determined by combining data acquired at different diffraction conditions and analyzing the black-white contrast orientation with respect to the set diffraction vector. Validation against expert manual evaluation shows a detection accuracy of 94% and a classification accuracy of 79%. These results demonstrate that Revelios SW prototype provides a robust and scalable solution for high-throughput GaN defect metrology and could be suitable for epitaxial process optimization and manufacturing control. Automation significantly increases throughput and reliability, supports efficient quantitative TD analysis, and makes the methodology accessible to less experienced users.

04

Classical semiconductors

MONDAY · 31 AUGUST 2026

17:00–18:20

Hall of Mirrors

Chair: Martien den Hertog

PRESENTATIONS

- 04.1 Jose Luis Pura**
InP/InGaP axially heterostructured nanowires for tandem solar cells studied by sub-micrometric optical characterization techniques
- 04.2 Muskan Jain**
Profiling Electrically Active Defects in AlGaInP by Impedance Spectroscopy
- 04.3 Xinyu Lv**
In-rich defect structures in InAs single crystals revealed by transmission electron microscopy
- 04.4 Ginés González-Guirado**
Nanoscale characterization of stress in Si nanowires for semiconductor qubit fabrication

InP/InGaP axially heterostructured nanowires for tandem solar cells studied by sub-micrometric optical characterization techniques

T. Van Tan^{1,2}, G. González-Guirado¹, L. Hrachowina³, M.T. Borgström³, J.L. Pura¹, J. Jiménez¹, O. Martínez^{1,*}

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Semiconductor nanowires (NWs) offer unique electronic and optical properties, such as tunable band-gaps, electromagnetic confinement, and relaxed lattice mismatch conditions, which promise to surpass mature planar technologies. Their capability for elastic mismatch accommodation enables the creation of high-performance axial heterostructures for applications in optoelectronic devices. Intensive research is required to overcome challenges such as abrupt heterojunctions and doping profiles. In this regard, micro- and nano-scale characterization techniques are essential for providing growth feedback, monitoring the composition, strain, or doping of the NWs. Contactless optical spectroscopies, such as photoluminescence (PL) and Raman, offer critical insights into the properties of the NWs.

In this study, tandem n-i-p InP/In_xGa_{1-x}P NWs connected by an Esaki diode were deposited on silicon substrates coated with different metals (Au, Ir, or Cr) to tailor charge transfer and heat dissipation during light exposure for optical measurements. The NWs were studied in plan-view, oriented both parallel (||) and perpendicular (⊥) to the polarization of the laser light, observing important differences related to the electromagnetic enhancement of the Raman/PL signal. The NWs response shows nearly dipolar nanoantenna resonances, i.e. maximum signal when the incident field is polarized along its axis. One of the main goals of the study was to deduce the best conditions for the sub-micrometric analysis of the NWs, to characterize the different sectors of the heterostructure. We pay special attention to the tunnel diode region, which demands a sharp interface with a narrow space charge region to allow effective tunneling.

Fig. 1 shows representative μ -PL and μ -Raman spectra taken along a NW ([Ga]=0.68 in the top cell, 6 μ m long). The peak intensities, positions and FWHMs of both PL and Raman spectra vary along the NW length according to the local composition, strain and doping. Regarding the PL data, for instance, localized variations in the InP bandgap due to doping and strain can be clearly observed (see the variation of the double band peak at $\sim$ 830 and $\sim$ 880 nm). On the other hand, Raman spectra of the InGaP region are very sensitive to the local Ga content. Note the high Raman intensity at the p⁺⁺-InGaP side of the tunnel diode, which allows us to identify this very narrow region, while the n⁺⁺-InP side of the tunnel diode appears to be Raman blind, because of the electromagnetic rejection in this region of the NW. μ -PL and μ -Raman are thus powerful techniques for studying different features of axially heterostructured NWs. And even though the spatial resolution along the NW axis is compromised by the diffraction limit, the optical resonances observed at different regions allow us to place their positions and extract additional information.

Improved spatial resolution using Raman and PL techniques is required for a fine analysis of the HJs. This can be achieved by using tip enhanced Raman and PL (TERS/ TEPL). This kind of measurements are now in progress and will be discussed in the final work.

Acknowledgments

This work has been funded by MICIU/AEI/ 10.13039/501100011033 and by “ERDF/EU”, under projects PID2023-148369OB-C43 and PID2024-157972OA-C22.

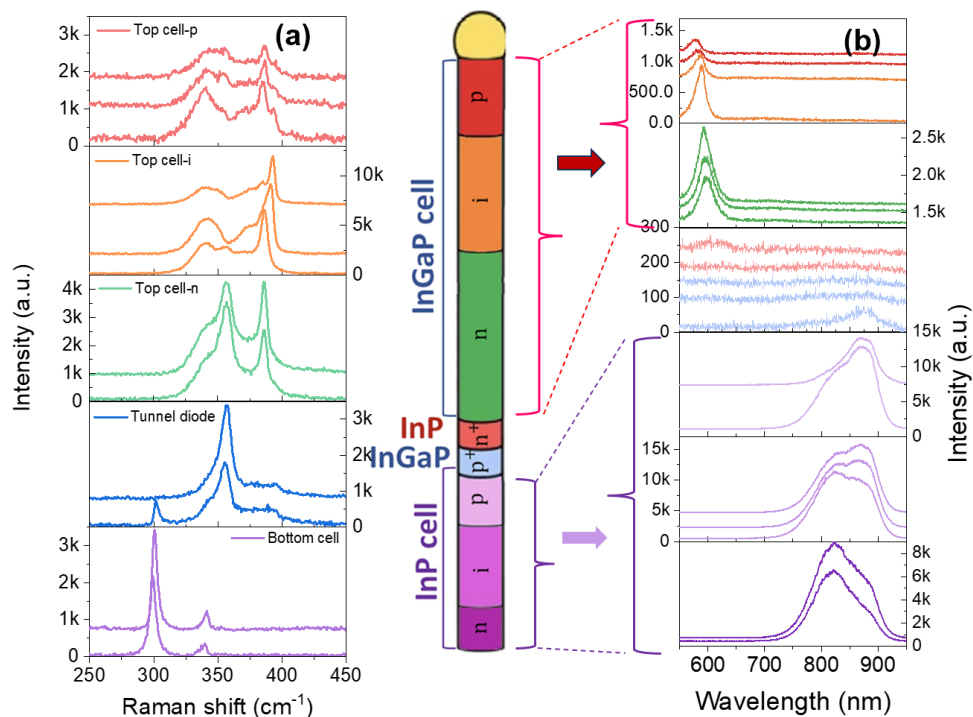


Figure 1: Representative μ -Raman (a) and μ -PL (b) spectra corresponding to the bottom cell, tunnel diode and top cell regions, taken along a line profile (step = 100 nm) along an InP/In_{0.32}Ga_{0.68}P NW, for an electric field polarization parallel to the analysed NW.

Profiling Electrically Active Defects in AlGaInP by Impedance Spectroscopy

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Miniaturized AlGaInP-based red micro-LEDs exhibit a pronounced efficiency degradation compared with their large-area counterparts, despite internal quantum efficiencies exceeding 90% in conventional LEDs. This “size effect” is widely attributed to non-radiative recombination centers generated near mesa sidewalls and semiconductor–insulator interfaces during fabrication and passivation [1,2]. However, the physical origin, distribution, and electrical activity of these defects remain insufficiently understood.

In this work, electrically active defects in $(\text{Al}_x\text{Ga}_{1-x})_{0.5}\text{In}_{0.5}\text{P}$ alloys ($x = 0, 0.5, 0.8, 1$) are investigated using planar metal–oxide–semiconductor (MOS) test structures that emulate the semiconductor–insulator interface present in micro-LED sidewalls (Fig. 1). Multi-frequency capacitance–voltage (CV) and conductance–voltage (GV) measurements were performed using a Keysight E4980 LCR meter across 100 Hz–1 MHz in frequency-sweep mode to capture full spectra at each bias, enabling detailed analysis of trap dynamics and interface states.

The CV characteristics of the $(\text{Al}_{0.5}\text{Ga}_{0.5})_{0.5}\text{In}_{0.5}\text{P}$ MOS structure measured at 295 K show pronounced non-ideal behaviour (Fig. 2). At 1 MHz, the capacitance saturates at ~20% of the nominal oxide capacitance ($C_{\text{ox}} \approx 0.005 \text{ F/m}^2$), indicating that true accumulation is not achieved even under strong forward bias up to +8 V (Fig. 3). This behaviour suggests the presence of an additional series capacitance originating from a persistent semiconductor depletion layer. The effect is attributed to strong surface potential pinning caused by a high density of near-interface defect states at the AlGaInP/Al₂O₃ interface.

The CV response also exhibits significant frequency dispersion at room temperature, indicating carrier exchange between the semiconductor and border traps in the Al₂O₃ layer. This dispersion is strongly reduced at lower temperatures (Fig. 4) due to decreased trap capture and emission rates [3]. To interpret these observations, physics-based TCAD simulations using Ginestra™ were performed [4]. The simulations indicate a surface-pinning level located ~0.3 eV below the conduction band minimum in $n\text{-(Al}_{0.5}\text{Ga}_{0.5})_{0.5}\text{In}_{0.5}\text{P}$ (Fig. 5). A complementary error-function trap distribution extending ~5 nm into the semiconductor (Fig. 6) reproduces the measured CV and GV characteristics (Fig. 7). Similar trend was exhibited by all material compositions and will be discussed (Fig. 8).

In summary, we have conducted the preliminary analysis of electrically active defects in the AlGaInP MOS system with different Al/Ga relative content. The experimental results, along with TCAD simulations, reveal a high density of traps near the AlGaInP/Al₂O₃ interface. The associated surface potential pinning explains the persistent semiconductor depletion even under high forward biases.

References

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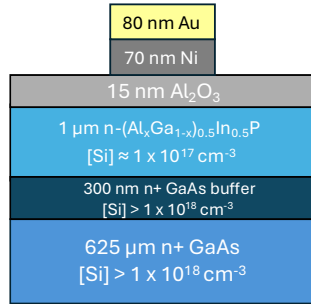


Fig. 1: Cross-sectional schematic representation of the n-GaAs/n-AlGaInP/Al₂O₃/Ni/Au MOS structure. 1 μm Si-doped AlGaInP layer was grown on n⁺-GaAs substrate by MOVPE. 15 nm Al₂O₃ dielectric layer was deposited by ALD, followed by Ni/Au (70/80 nm) gate stack deposition using e-beam evaporation.

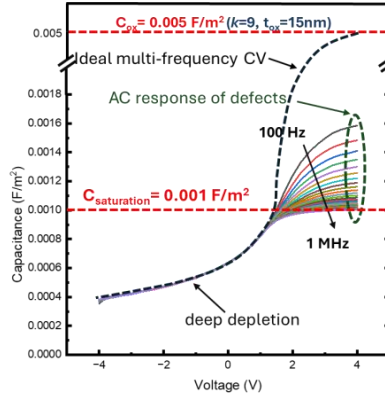


Fig. 2: Multi-frequency CV response for n-doped (Al_{0.5}Ga_{0.5})_{0.5}In_{0.5}P MOS structure at RT in a dark and dry air environment.

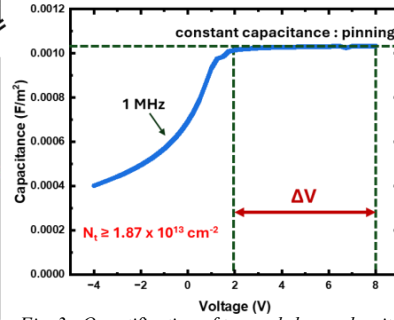


Fig. 3: Quantification of trapped charge density near n-doped (Al_{0.5}Ga_{0.5})_{0.5}In_{0.5}P/Al₂O₃ interface by high frequency (1 MHz) CV measurement in extended positive bias region at RT in dark and dry air environment.

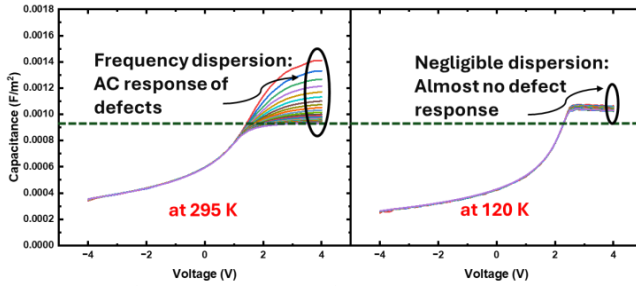


Fig. 4: Multi-frequency CV responses for n-AlInP MOS structure measured at 295 K and 120 K in dark. Frequency dispersion, which is related to the AC response of border traps interacting with majority charge carriers, becomes negligible at 120 K due to suppressed capture and emission rates of border traps.

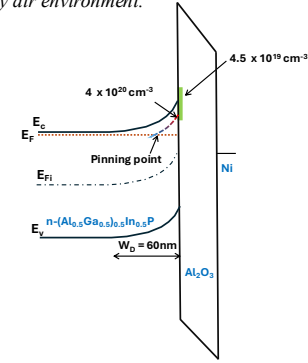


Fig. 5: Distribution of trap densities used for simulating n-(Al_{0.5}Ga_{0.5})_{0.5}In_{0.5}P/Al₂O₃ MOS system. The trap level is located 0.3 eV below E_c with density decaying rapidly into the semiconductor.

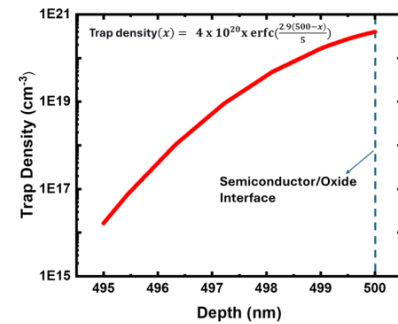


Fig. 6: Distribution of trap density in (Al_{0.5}Ga_{0.5})_{0.5}In_{0.5}P used for simulations. The distribution follows complementary error function, and the trap density drops significantly within 5 nm from the interface. The integrated trap density is $4 \times 10^{13} \text{ cm}^{-2}$ (in agreement with the value obtained in Fig. 3).

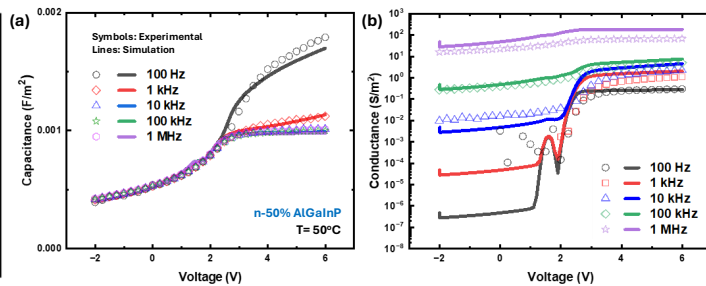
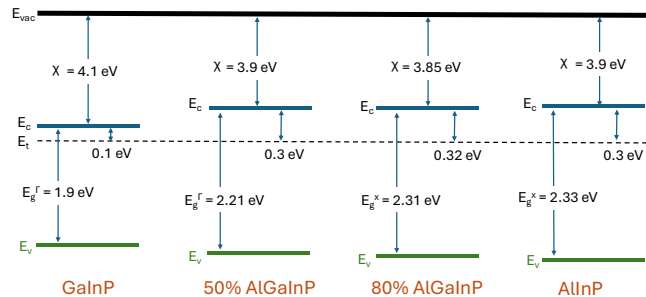


Fig. 7: Multi frequency (a) CV and (b) GV response of n-(Al_{0.5}Ga_{0.5})_{0.5}In_{0.5}P/Al₂O₃ MOS system at 50°C: experimental data (symbols) and simulated response (lines) including traps in oxide and AlGaInP (as shown in Fig. 5 and 6).

Fig. 8: Distribution of the pinning trap levels (E_t) across different composition systems, as obtained from experimental results and TCAD simulations. For different compositions, the trap levels were found to be at similar energy levels with respect to the vacuum level.



In-rich defect structures in InAs single crystals revealed by transmission electron microscopy

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Indium arsenide (InAs) serves as a key substrate material for infrared optoelectronics. The performance and yield of infrared optoelectronic devices are influenced by defects in substrates. While dislocations, stacking faults, and twins are commonly observed in melt-grown crystals, transmission electron microscopy (TEM) studies focusing on nanoscale defects remain limited [1-2]. Investigating these nanoscale defects is therefore essential, as it enables precise identification of defect types, reveals the microscopic mechanisms of nucleation and evolution, and establishes critical relationships among growth processes, microstructures, and material properties.

A 2-inch, (100)-oriented, non-doped InAs substrate was used in this study. To eliminate surface damage, approximately 200 μm was uniformly removed from its surface using a chemical etchant ($\text{H}_3\text{PO}_4\text{:H}_2\text{O}_2 = 1\text{:}1$). A cross-sectional specimen along the [110] direction was then prepared by focused ion beam (FIB) milling for subsequent TEM characterization of growth defects. As shown in Figure 1, conventional TEM bright-field imaging reveals stacking faults, moiré fringes and numerous randomly distributed regions exhibiting abnormal contrast. These regions are considered characteristic defects formed during InAs single-crystal growth. High-resolution TEM imaging of several such defects reveals similar microstructural features. The corresponding diffraction patterns consistently exhibit a ring of secondary spots surrounding each primary diffraction spot. Energy-dispersive X-ray spectroscopy (EDS) mapping further rules out impurity contamination as the origin of these defects. These observations suggest that the defects arise from lattice deformation with a certain regularity during crystal growth. Given that conventional TEM could not resolve the fine microstructure of these defects, spherical aberration-corrected TEM (Cs-corrected TEM) is employed for further analysis. As shown in Figure 2, EDS line scans across the first type of defect reveal In enrichment and As depletion within the defect region. Concurrently, the spacing of the (111) lattice planes in this region is significantly reduced. These findings suggest that the formation of this defect type may be associated with As volatilization during crystal growth, possibly leading to localized In accumulation in a manner resembling insertion-type stacking faults. Figure 3 presents the analysis of the second defect type. While this type also exhibits In enrichment and As depletion, no reduction in lattice spacing or additional spots in the electron diffraction pattern is observed. These results demonstrate that precise control of the III/V element ratio is essential during III–V single-crystal growth.

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Acknowledgment

This work is partially supported by the National Key R&D Program of China (Grant Nos. 2025YFF0511902, 2024YFA1208901), the National Natural Science Foundation of China (Grant Nos. 52401250, 62374161).

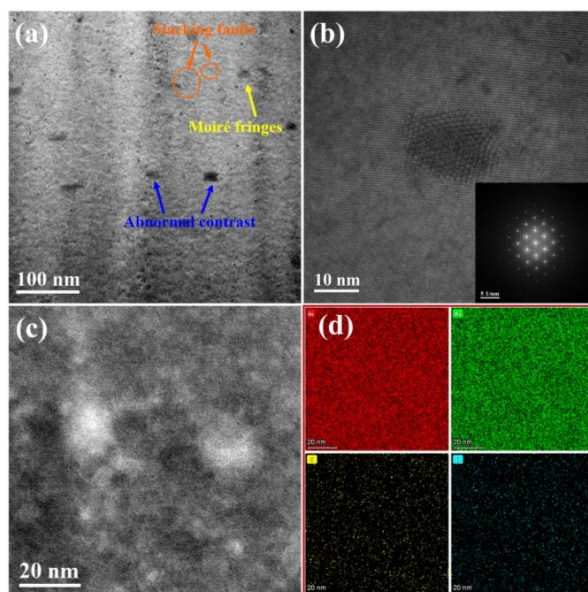


Figure 1. (a) TEM bright-field image of a $[110]$ -oriented cross-sectional specimen; (b) high-resolution TEM image and corresponding electron diffraction pattern of regions exhibiting abnormal contrast; (c) high-angle annular dark-field (HAADF) image of the abnormal contrast regions; (d) EDS elemental maps of In, As, C, and O from the area shown in (c).

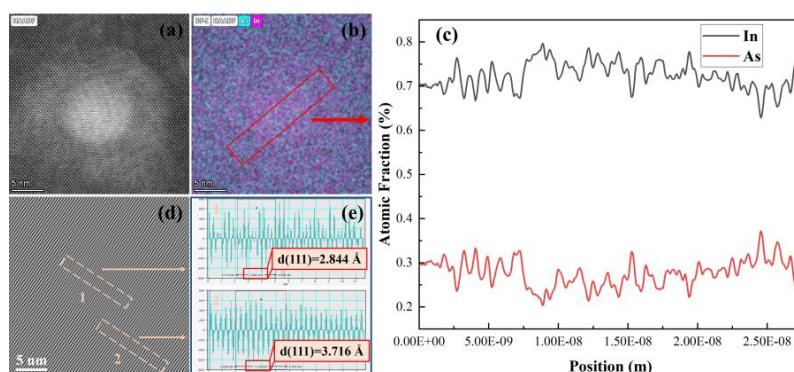


Figure 2. Characterization of type I defects exhibiting abnormal contrast. (a) HRTEM image acquired by aberration-corrected TEM; (b) corresponding EDS elemental maps of In and As; (c) EDS line scan across the region indicated by the red box in (b); (d) lattice fringe image of the (111) planes corresponding to the area in (a); (e) measured (111) d-spacings for regions 1 and 2 marked in (d).

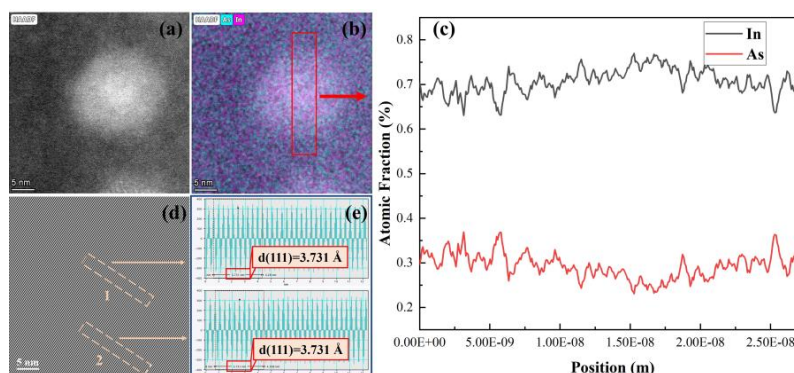


Figure 3. Characterization of type II defects exhibiting abnormal contrast. (a) HRTEM image acquired by aberration-corrected TEM; (b) corresponding EDS elemental maps of In and As; (c) EDS line scan across the region indicated by the red box in (b); (d) lattice fringe image of the (111) planes corresponding to the area in (a); (e) measured (111) d-spacings for regions 1 and 2 marked in (d).

Nanoscale characterization of stress in Si nanowires for semiconductor qubit fabrication

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The advancement of quantum computing technologies requires the scalable development of reliable qubit platforms. One of the most promising strategies to address this challenge involves adapting current silicon nanoelectronic technology to meet the requirements for the fabrication of semiconductor-based qubits. In this context, Si nanowires (NWs) are particularly attractive for realizing spin-based qubits in fully depleted silicon-on-insulator (FD-SOI) platforms [1]. The performance of quantum devices is critically dependent on the quality of the materials. Factors such as the presence of crystalline disorder, the state of the surface, or modifications caused during the device processing dramatically influence their performance and reliability. In this work, we report a micro-Raman spectroscopy investigation of Si NWs fabricated by dry etching on FD-SOI wafers, aimed at assessing the presence of residual stress.

The samples are composed of a bulk Si substrate, a 400 nm layer of buried oxide (BOX) SiO₂, and a 50 nm layer of monocrystalline Si. The NWs (50 nm in width) and their source/drain connections were defined on the top Si layer using a mix-and-match lithography approach combining electron-beam and optical patterning, followed by dry etching. According to this structure, the Raman spectrum is dominated by the signal arising from the Si substrate, hindering the correct characterization of the Si NW. To overcome this challenge, we present two different methodologies. First, we intentionally induced localized laser heating of the NW with the incident beam to modify the Raman spectrum of the NW and distinguish it from the signal of the unperturbed Si substrate. This permits us to decouple the Raman signals of the Si NW and the substrate to extract the NW stress. Second, we locally removed the underlying bulk Si substrate and the BOX SiO₂ layer beneath several NWs to obtain free-standing Si NWs, enabling direct measurement of the Si NWs stress. These experimental measurements were supported by Finite Element Methods simulations to correctly analyze the stress profiles. We obtained comparable stress values with both methodologies (0.17-0.34 GPa), corresponding to small elastic strains (0.1-0.2%), albeit enough to lift the heavy-hole/light-hole degeneracy and reduce band mixing [2]. These modifications could favor hole-qubit operation while remaining well below mechanical stability thresholds. The results confirm the suitability of the etching process for fabricating Si NW-based qubits and establish a reliable platform for a robust non-invasive characterization, even under unfavorable experimental conditions.

References

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Acknowledgments

The authors acknowledge the financial support from grants PID2021-126046OB-C21, PID2021-126046OB-C22, and PID2024-157972OA-C22 funded by MICIU/AEI/10.13039/501100011033 and “ERDF/EU”, grant TED2021-130786B-I00 funded by NextGenerationEU/PRTR, and the “María de Maeztu Unit of Excellence” (CEX2023-001397-M). JLS acknowledges support from the grant RYC2023-043765-I, and the Trigger project INSPECTOR; JAL thanks the Generation D initiative; GGG acknowledges the financial support of Junta de Castilla y León through a predoctoral fellowship.

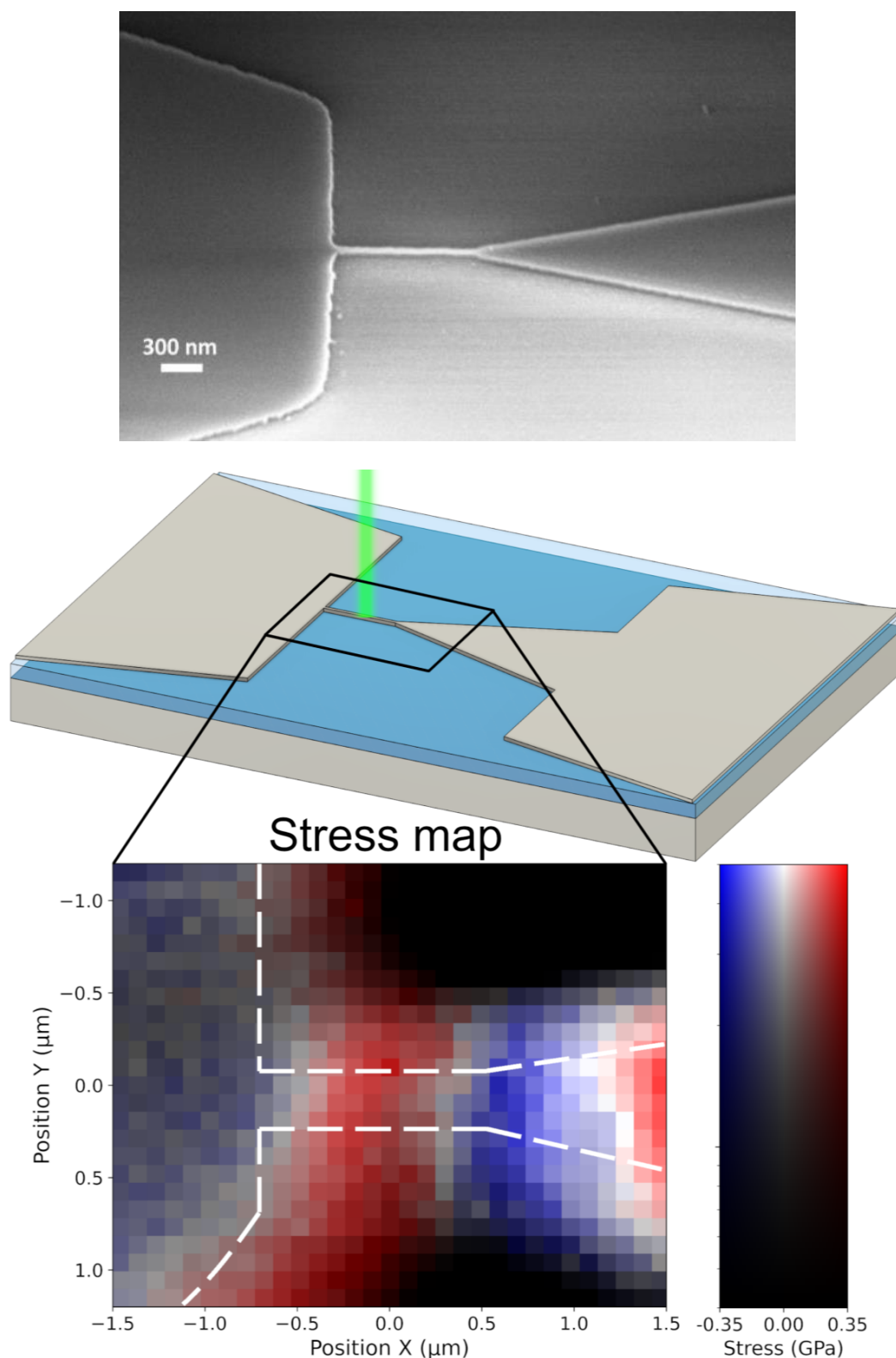


Figure 1: SEM image of a Si NW and its source/drain connections. Schematic representation of the sample and the laser beam. Experimental stress map corresponding to the optical image. The contour of the structure is drawn with white dashed lines. The intensity of the colorbar (vertical) represents the Raman integrated area on a log scale, while the color scale (horizontal) encodes the calculated stress in GPa: blue indicates compressive stress, white indicates zero stress, and red indicates tensile stress.

05

III-nitrides I

TUESDAY · 1 SEPTEMBER 2026

08:50–10:30

Hall of Mirrors

Chair: Anna Kaleta

PRESENTATIONS

- 5.0** **Carsten Richter** INVITED
3D Characterization of Dislocation Development in Seeded Growth of AlN Bulk Crystals
- 05.1** **Kazuki Ohnishi**
Examination of Burgers vectors of dislocations in GaN substrates via reflection and transmission synchrotron X-ray topography
- 05.2** **Domenik Spallek**
Distortion tensor around individual dislocations in GaN studied by electron backscatter diffraction and cathodoluminescence spectroscopy
- 05.3** **Aaron Holmes**
Deep Learning of Dislocations in GaN: From Detection to Spatial Analysis

3D Characterization of Dislocation Development in Seeded Growth of AlN Bulk Crystals

M.P. Kabukcuoglu², C. Hartmann¹, M. Albrecht¹, M. Bickermann¹,
E. Hamann², M. Hurst², C. Yildirim³, D. Hänschke², T. Straubinger¹ and C. Richter^{1*}

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Aluminum nitride (AlN) is a critical substrate material for deep ultraviolet optoelectronics, high-power electronics, and sensor applications. Next to challenges related to n-type doping of AlN, the lack of high-quality crystals with diameter of 4 inches or more is currently hindering a widespread exploitation of this material in semiconductor industry. In the development of crystals with larger diameters and volume, maintaining a sufficient supply of source material and low thermal gradients becomes increasingly challenging. However, controlling these parameters is crucial to limit the formation of crystal defects, such as grain boundaries and dislocations, thereby preserving high crystal quality.

Our work aims at understanding the evolution of defects, in particularly dislocations, during seeded growth of AlN crystals and their diameter-increase by growth on different crystallographic surfaces. We investigated the behavior of dislocations during regrowth on the seed using 2D and 3D X-ray diffraction imaging and complementary techniques, enabling us to determine the direction and sense of the Burgers vectors, as well as dislocation line trajectories in 3D.

While parts of the dislocations are inherited from the seed, they typically exhibit a strong lateral displacement at the seed to bulk interface.

In crystals grown at a relatively small lateral temperature gradient, dislocations bend near the seed interface (see Fig. 1), with their movement governed by a climb process. The absence of slip was inferred from the Burgers vector orientation in relation to the movement direction and can be explained by a low resolved shear stress that is insufficient to activate glide. In contrast, the climb process is facilitated by a significant level of oxygen impurities, and becomes the dominating mechanism of motion during growth at low temperature gradients (0.1 K/mm) [1].

When growing at larger lateral temperature gradients, the crystals diameter increases rapidly [2], leading to enhanced nucleation of dislocations at the $\langle 1\bar{1}00 \rangle$ corners and glide towards the center of the crystal [3]. Dislocations from the seed, however, are partially deflected at the regrowth interface and cannot penetrate into the bulk (see Fig. 2) as shown by 3D imaging data.

These findings demonstrate how the temperature field can be used to control defect formation in AlN substrates and how 3D X-ray diffraction imaging enables insights into the history of dislocation formation, which can be related to the growth processes in these crystals.

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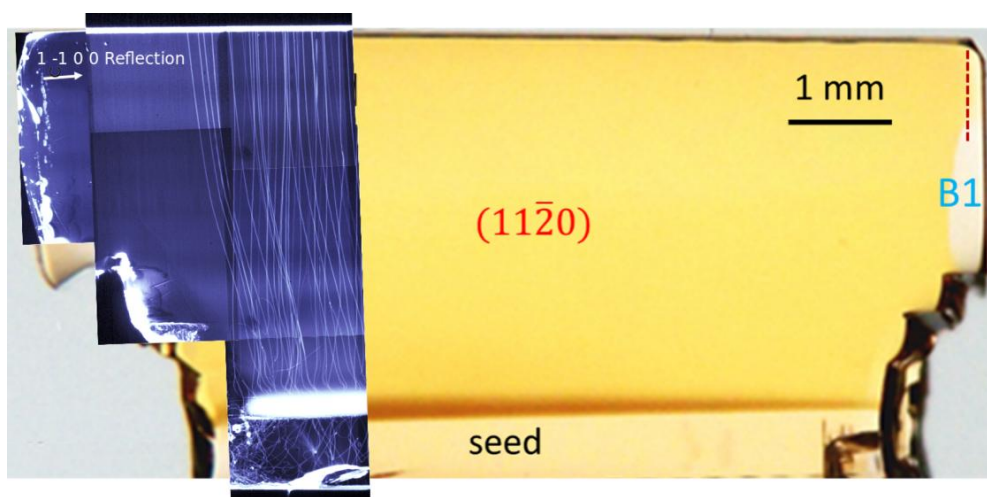


Figure 1: Monochromatic beam X-ray topography image of the $1\bar{1}00$ Bragg reflection from a $(11\bar{2}0)$ AlN wafer overlaid on a photograph of the wafer. The seed to bulk interface exhibits a high mosaicity and strong bending of dislocations that are inherited from the seed.

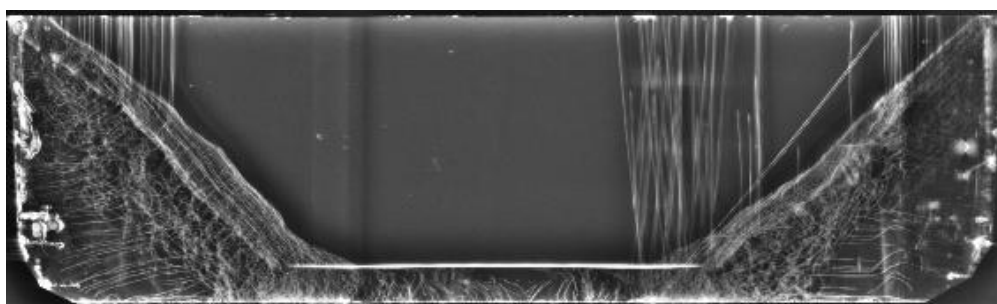


Figure 2: White beam X-ray topography image of the $11\bar{2}0$ Bragg reflection of a $(1\bar{1}00)$ AlN wafer. Some dislocations are inherited from the seed, while others are deflected at the seed to bulk interface.

Examination of Burgers vectors of dislocations in GaN substrates via reflection and transmission synchrotron X-ray topography

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To improve the performance and reliability of vertical GaN power devices, it is crucial to identify killer defects and elucidate their spatial distribution in GaN substrates. X-ray topography (XRT) is a powerful nondestructive technique for characterizing dislocations and their Burgers vectors (**b**) over a wide area. While most previous XRT studies on GaN substrates have employed the reflection geometry [1], this configuration limits observations to near-surface regions. Transmission XRT under the Borrmann effect enables direct observation of dislocation propagation in thick substrates [2, 3]; however, image interpretation, including reliable **b** determination, is complicated by dynamical diffraction and non-vertical dislocation propagation in GaN. In this study, reflection and transmission XRT were combined to estimate the **b** of dislocations in GaN substrates.

A GaN substrates grown by the acidic ammonothermal growth method was investigated. Synchrotron XRT measurements were performed using reflection and transmission geometries at the BL-3C beamline of the Photon Factory, KEK and the BL24XU beamline of SPring-8, respectively. Diffracted and forward-diffracted beams were recorded using a X-ray film and a CMOS digital camera.

Figure 1 shows reflection XRT images obtained with six equivalent **g** vectors of $\mathbf{g} = 11\bar{2}4$. Labeled threading dislocations (TDs) exhibited bright and dark contrasts, indicating that these TDs are edge- or mixed-type dislocations. However, precise identification of their **b** was difficult due to the limited spatial resolution of the X-ray film. Bright-field transmission XRT images were performed by recording forward-transmitted waves with three **g** vectors. The contrasts of E1, E2, E3, and M1 were nearly invisible for $\mathbf{g} = 01\bar{1}0$, whereas M2 remained visible for all measured **g** vectors. These results suggest that E1, E2, E3, and M1 have *a*-components of **b** parallel or antiparallel to $[2\bar{1}\bar{1}0]/3$, while the **b** of M2 could not be determined from $\mathbf{g} \cdot \mathbf{b}$ invisibility criterion alone. Because the **b** of M2 could not be determined from the $\mathbf{g} \cdot \mathbf{b}$ invisibility criterion alone, the linewidths under off-Bragg conditions were analyzed, where the width is proportional to $\sqrt{|\mathbf{g} \cdot \mathbf{b}|}$ due to a kinematically scattering [3]. By comparing the experimental linewidths and the calculated values, the **b** of TDs were estimated (Table 1). Although the estimated **b** of M2 ($[11\bar{2}\bar{3}]/3$) is orthogonal to the applied **g** vector $\bar{1}100$, its contrast was faintly visible. This is presumably due to residual lattice distortion caused by the surface relaxation effects and/or the condition $\mathbf{g} \cdot (\mathbf{b} \times \mathbf{l}) \neq 0$, where **l** is the direction vector of the dislocation line. These results demonstrate that combining reflection and transmission XRT enables more reliable estimation of **b** in GaN substrates, improving dislocation analysis.

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Acknowledgment

We would like to thank Professor Keiichi Hirano with the at the High Energy Accelerator Research Organization (KEK) for his support in maintaining the BL-3C beamline at the Photon Factory.

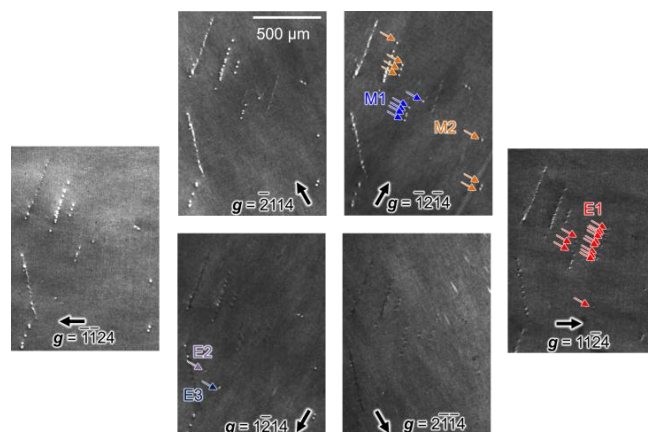


Figure 1: Reflection XRT images taken with the six-equivalent $\mathbf{g}$ vectors of $11\bar{2}4$. TDs labeled exhibited bright and dark contrasts depending on the $\mathbf{g}$ vector.

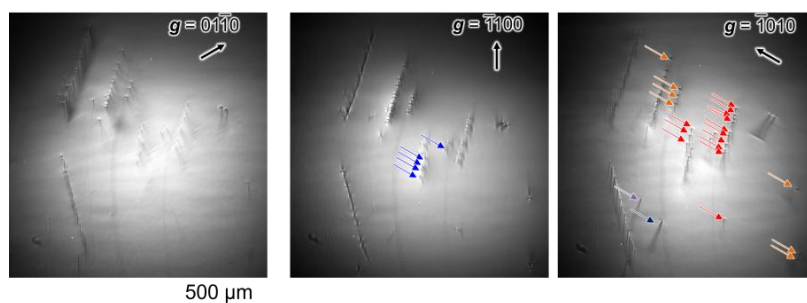


Figure 2: Transmission XRT images taken from the same area as shown in Figure 1 using the forward-transmitted wave with $\mathbf{g} = 01\bar{1}0$, $\bar{1}100$, and $\bar{1}010$.

Table 1: Estimated $\mathbf{b}$ of E1, E2, E3, M1, and M2.

	E1	E2	E3	M1	M2
$\mathbf{b}$	$[2\bar{1}\bar{1}0]/3$	$[\bar{2}110]/3$	$[\bar{4}220]/3$ or $[\bar{6}330]/3$	$[2\bar{1}\bar{1}\bar{3}]/3$	$[11\bar{2}\bar{3}]/3$

Distortion tensor around individual dislocations in GaN studied by electron backscatter diffraction and cathodoluminescence spectroscopy

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The local change of the bandgap caused by the elastic distortion in the vicinity of a threading dislocation (TD) in GaN has been evidenced by luminescence spectroscopy mapping in multiple cases [1]. However, experimentally quantifying this distortion and its components remains a challenge due to the expected low amplitudes in the range of 10^{-3} for strains [2].

In this study, a c-plane, homoepitaxial GaN-layer, grown by molecular beam epitaxy on a freestanding substrate, is investigated. The TD density was determined to be lower than 10^6 cm^{-2} and these are predominantly of mixed- and edge-type according to XRD measurements.

Individual dislocations were identified using cathodoluminescence (CL) mapping and high-resolution electron backscatter diffraction (HR-EBSD). Maps were recorded for more than 10 dislocations with an EDAX Clarity direct detection EBSD system. On $2 \times 2 \mu\text{m}^2$ maps with step sizes of 30 nm, the dislocations are well resolved by maxima of 0.7 mrad in the Kernel Average Misorientation (KAM) that otherwise shows statistical noise of 0.16 mrad.

The Kikuchi patterns were further analyzed by cross-correlation analysis using the Software CrossCourt from BLG Vantage [3] to calculate all components of the spatially-resolved distortion tensor. Reference measurements on a freestanding substrate in a dislocation-free area were used to quantify the sensitivity to 5×10^{-4} for strains and 0.3 mrad for rotations. This sensitivity is high enough to identify signatures of the dislocation, e. g. peaks/sinks or dumbbell-shapes, in strain and rotation components. The experimental maps were compared with the calculations of the distortion tensor components at the surface, taking into account the strain relaxation at the surface. Since it is possible to relate the experimental results to these calculations and different dislocation types have distinguishable signatures, the Burgers vectors can be derived. Following this approach, a neighboring pair of dislocations with opposite Burgers vectors was observed.

Finally, hyperspectral cathodoluminescence (CL) maps were recorded in a UV-optimized setup around the same individual dislocations with the same spatial resolution. As expected, the maps reveal a reduced intensity as well as a shift of the near-bandedge emission energy on a scale of $\pm 2 \text{ meV}$ at room temperature.

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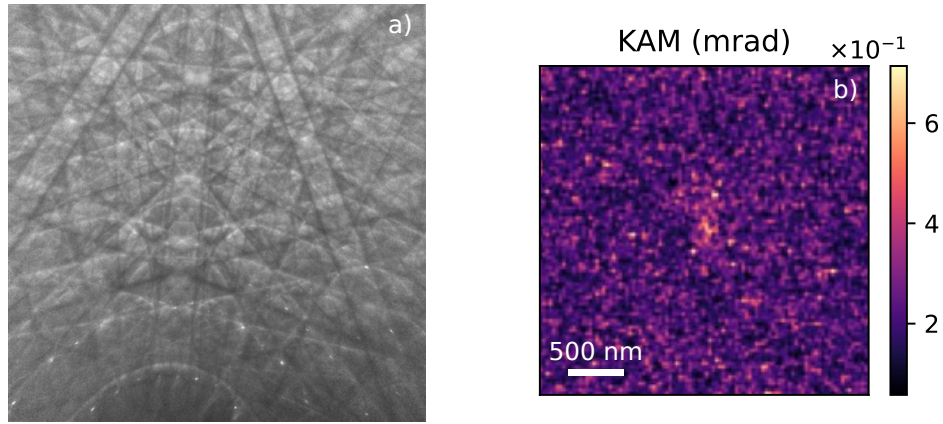


Figure 1: a) Representative Kikuchi pattern obtained from HR-EBSD on the homoepitaxial GaN-sample, b) Kernel Average Misorientation (KAM) map around an individual dislocation obtained from spherical indexing of the Kikuchi patterns.

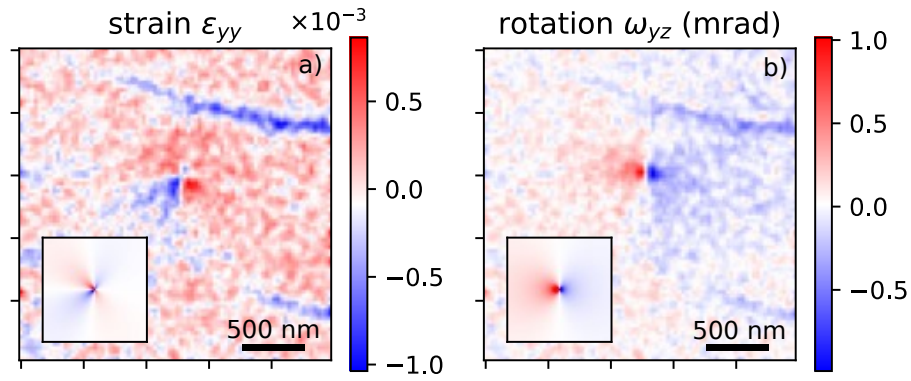


Figure 2: Selected distortion tensor components around an individual mixed-type dislocation a) ϵ_{22} b) ω_{23} , insets show calculations for this type of dislocation.

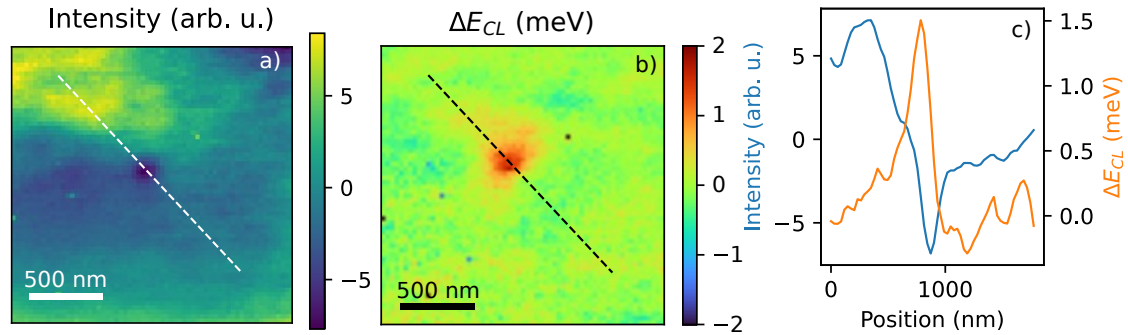


Figure 3: a) Intensity and b) spectral shift of the Gaussian component of the fit to the hyperspectral CL map recorded around the same dislocation as in Figure 2, c) Profiles of intensity and spectral shift along the dashed lines in a) and b).

Deep Learning of Dislocations in GaN: From Detection to Spatial Analysis

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Dislocations in Gallium Nitride (GaN) significantly impact the performance of devices [1, 2], making accurate quantification essential. To visualise these defects, a technique called Electron Channelling Contrast Imaging (ECCI) can be used. ECCI is a non-destructive Scanning Electron Microscopy (SEM) technique that uses variations in backscattered electron yield due to changes in strain and orientation, making individual dislocations appear as distinct black-white contrast spots [3]. While ECCI allows us to observe these defects across large areas, identifying them manually is slow and inconsistent. This limits our ability to analyse materials with high throughput. To address this, we develop and compare three automated methods for detecting dislocations in ECCI.

We have tested a rule-based computer vision approach, a multi-stage Convolutional Neural Network (CNN), and a unified single-stage detector (YOLOv8 [3]). Evaluated against repeated manual counting, the rule-based method struggled with varying ECCI contrast, and the CNN was computationally slow (hours per image). However, YOLOv8 proved highly effective, achieving $98.9 \pm 1.1\%$ raw counting accuracy and reducing processing time to tens of seconds. Crucially, we found that a confidence threshold of 0.025—ten times lower than typical validation choices [4]—optimised detection for faint dislocations without increasing false positives, yielding 99.2% precision, 98.1% recall, and a 98.6% F1 score across a test set of 4361 dislocations.

Beyond simple density calculations, this rapid detection enables statistical analysis of defect spatial relationships. GaN dislocations frequently self-organise into linear arrays or trace low-angle grain boundaries. By analysing the coordinates of detected defects, we aim to quantify local ordering. Distinguishing randomly distributed defects from organised networks provides deeper insights into the material's structural evolution and relaxation state.

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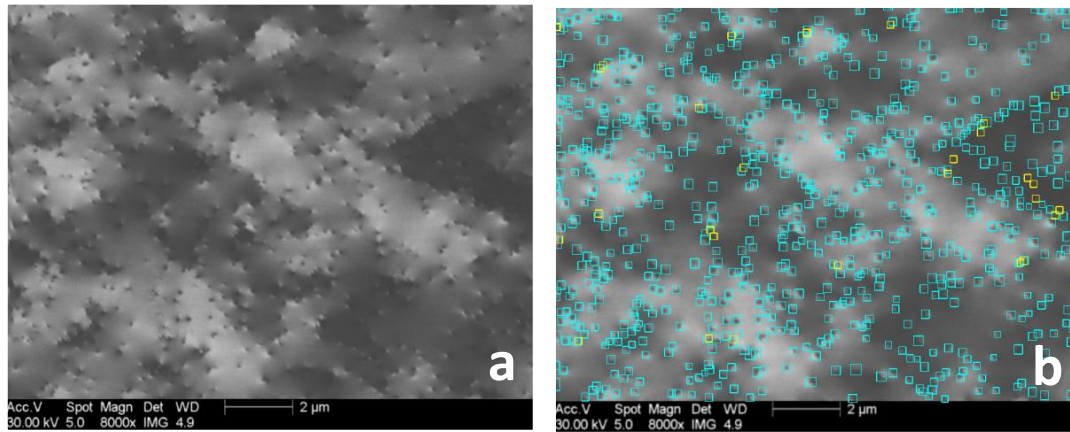


Figure 1: Detection performance on a benchmark GaN ECCI micrograph. (a) Original image containing 730 ± 8 dislocations. (b) Automated YOLOv8 detections shown in cyan, with manual corrections (missed dislocations) highlighted in yellow. Achieving 98.9% precision, 96.2% recall, and an F1-score of 97.5%. In total, 36 manual edits (8 false positives removed, 28 false negatives added) [5]

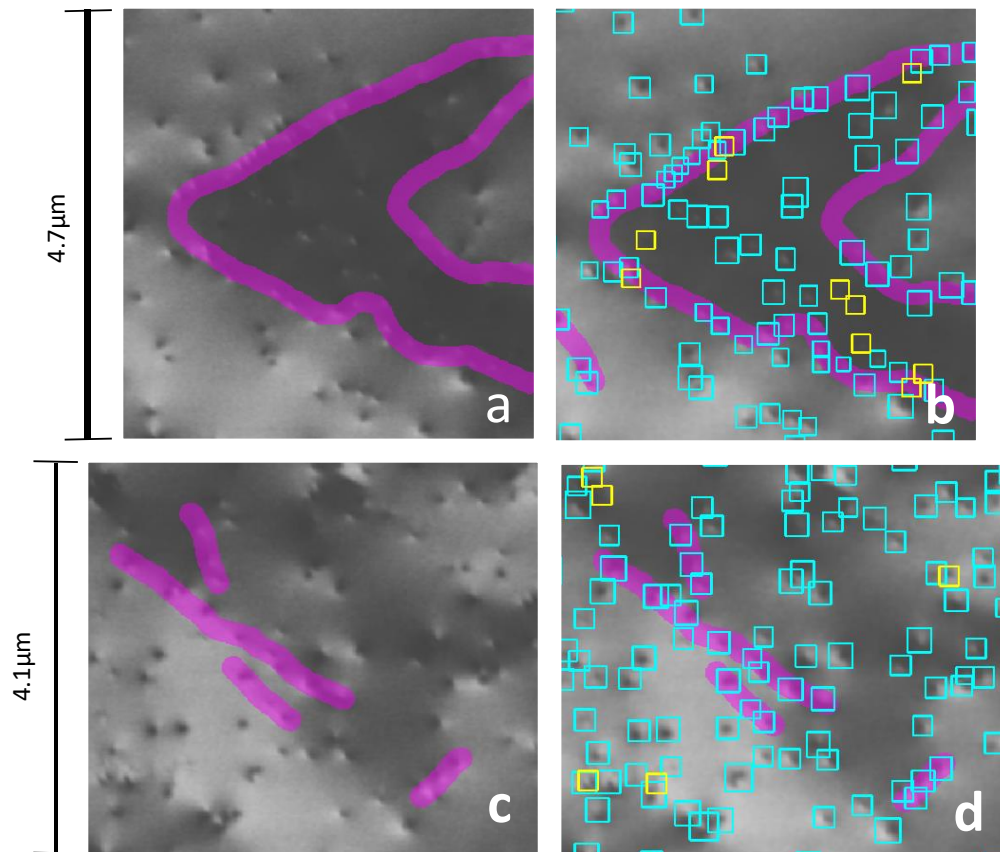


Figure 2: Evidence of dislocation organisation. (a, b) A low-angle grain boundary traced by a chain of dislocations. (c, d) Short linear arrays of dislocations. Images (a) and (c) include a purple overlay tracing these potential physical alignments. Images (b) and (d) show the corresponding detections. The features highlighted here suggest real structural self-organisation, which this high-throughput detection method now allows us to investigate. [5]

06

III-nitrides II

TUESDAY · 1 SEPTEMBER 2026

11:00–13:00

Hall of Mirrors

Chair: Takuo Sasaki

PRESENTATIONS

- 6.0** **František Hájek** INVITED
Ga Vacancy Diffusion at the Ammonothermal–MOVPE GaN Interface
- 06.1** **Roman Hrytsak**
Diffusion of Mg and Si dopants in the InGaN and AlGaN ternary alloys and throughout InGaN/GaN, AlGaN/GaN interfaces
- 06.2** **Lorenzo Rigutti**
Effects of Disorder and Stress on AlGaN multiple Quantum Well Structures studied by Photonic Atom Probe
- 06.3** **Magdalena Zając**
PEC etching of bulk ammonothermal Al_{0.06}Ga_{0.94}N: defect recognition in a ternary nitride alloy
- 06.4** **Bogdan Kowalski**
Mechanisms of increased luminescence of GaN nanowires covered with HfO_x shells

Ga Vacancy Diffusion at the Ammonothermal–MOVPE GaN Interface

František Hájek^{1*}, Jakub Čížek³, Pavel Eichler⁴, Robert Czernecki², Ewa Grzanka², Mike Leszczynski², Radek Fučík⁴, Jan Kuriplach³, Tomáš Hubáček¹, Pavel Hubík¹, Robert Kucharski², Tomasz Sochacki², Roman Hrytsak², Maciej Oskar Liedke⁵, Eric Hirschmann⁵, Andreas Wagner⁵, Alice Hospodková¹

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The stability and transport of native point defects at the interface between ammonothermally grown GaN substrates (containing large concentration of Ga vacancy-related complexes [1], [2]) and metal–organic vapor phase epitaxy (MOVPE) GaN epilayers are central to the performance and reliability of high-power and optoelectronic devices, yet remain insufficiently resolved. Here, we address the long-standing question of whether native vacancies formed in low-dislocation-density ammonothermal GaN can diffuse into subsequently grown MOVPE layers. We employ a complementary, depth-resolved methodology—combining Secondary Ion Mass Spectrometry (SIMS), capacitance–voltage (C–V) profiling, photoluminescence (PL), Raman spectroscopy, and variable-energy positron annihilation spectroscopy (VEPAS) with detailed drift–diffusion–trapping modeling—to map vacancy-type defect distributions with high sensitivity from the subsurface region into the bulk. Example of the VEPAS data modelling is shown in Fig. 1.

Unintentionally GaN epilayer grown at 930°C, H₂ atmosphere from TMGa precursor shows no evidence of Ga vacancy-related defect diffusion across the interface. Instead, several hundreds of nanometers inside the ammonosubstrate turns into the compensated layer after the epitaxy. This compensated layer electrically screens the substrate, effectively decoupling the epilayer in electrical measurements and establishing built-in electric fields that are expected to influence carrier transport, junction behavior, and device operating characteristics. Samples prepared at different growth conditions (temperatures, atmospheres) exhibit different behavior and the connection between the growth conditions and vacancy behavior will be discussed. The results are important for optoelectronic application including lasers, vertical p-n junctions or HEMTs.

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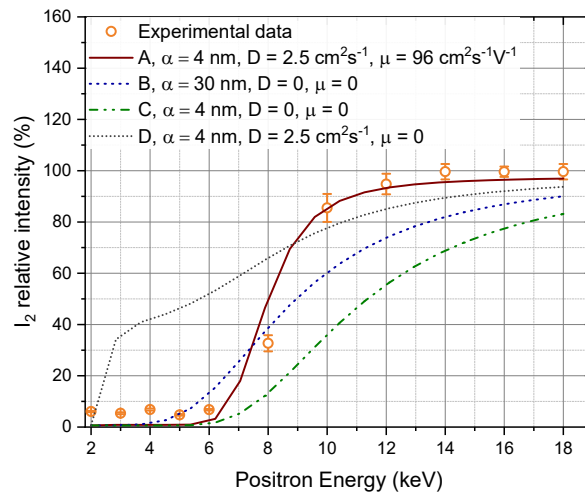


Figure 1: I_2 component of VEPAS decomposed spectra dependency on positron energy (GaN sample grown at 930°C in H_2 atmosphere). Solid lines are calculated in the frame of drift–diffusion–trapping model. Curve A – Ga vacancy related defects penetrate with characteristic length 4 nm, positron diffusion and drift are accounted, Curve B – Ga vacancy related defects penetrate with characteristic length 30 nm, positron diffusion and drift are not accounted, Curve C – Ga vacancy related defects penetrate with characteristic length 4 nm, positron diffusion and drift are not accounted, Curve D – Ga vacancy related defects penetrate with characteristic length 4 nm, positron diffusion is accounted but drift not.

Diffusion of Mg and Si dopants in the InGaN and AlGaN ternary alloys and throughout InGaN/GaN, AlGaN/GaN interfaces

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InGaN is a key wide bandgap semiconductor used as the active light emitting layer in blue, green, and white LEDs, laser diodes (LDs), and high power electronics. Its tunable direct bandgap allows for application not only in high efficiency solid-state lighting but also in micro-LED displays technology and superluminescent diodes (SLDs) where a wide emission spectrum and high output power is required. AlGaIn in turn, is essential for manufacturing UV-C LEDs, LDs and optical modulators due to its tunable bandgap, while AlGaIn/GaN heterostructures create high-electron mobility transistors (HEMTs) used in high-voltage rectifiers and converters, as well as solid-state sensors. The structural quality of both InGaIn/GaN and AlGaIn/GaN active regions, in particular interfacial morphology of the corresponding multi-quantum wells is crucial for any nitride-based device performance.

Herein, we performed DFT-based first principle calculations to study the diffusion of Mg and Si substitutional dopants in the $\text{In}_{0.02}\text{Ga}_{0.98}\text{N}$ and $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$ ternary alloys and the corresponding $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ and $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interfaces. We utilized a supercell model of the $\text{In}_x/\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys with the size $5 \times 5 \times 3$ and the diffusion was modelled using a vacancy-mediated mechanism. The diffusion paths of Mg and Si dopants were examined along the hexagonal c-axis, while the minimum energy migration paths were determined within the nudged elastic band (NEB) method. The heights of the migration energy barriers as well as the activation enthalpies were calculated taking into account a climbing-image refinement to the NEB relaxation results, as well as the vibrational free energy contribution in the harmonic approximation. To assess the influence of alloy composition and local coordination, we examined configurations of second-nearest-neighbor shell in $\text{In}_x\text{Ga}_{1-x}\text{N}$ and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ in which the Si or Mg dopant atom was surrounded by either single or three alloy atoms. Finally, we applied the harmonic transition-state theory to calculate the diffusion coefficients D_{Si} , D_{Mg} of migration Si and Mg dopants, both in neutral and charged states. Calculation results show that (i) the diffusion coefficients of magnesium and silicon are in general larger in $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$ than in $\text{In}_{0.02}\text{Ga}_{0.98}\text{N}$, both in a local surrounding of 1 and 3 In and Al alloy atoms, (ii) D_{Mg}^0 of neutral Mg dopant is larger than that of charged dopant D_{Mg}^{2+} , both in a local surrounding of 1 and 3 Al alloy atoms of AlGaIn, and the corresponding migration energy barrier lies in the range 1.67 – 1.73 eV, (iii) the situation is analogous for the neutral and charged Si dopant, only when it is surrounded by 1 Al alloy atom. In the case of 3 surrounding Al alloy atoms, the pre-exponential factor for $D_0(\text{Si}^{3-})$ of charged dopant equals $2.217 \text{ cm}^2/\text{s}$ and it is by one magnitude larger than that of neutral one, $D_0(\text{Si}^0) = 0.286 \text{ cm}^2/\text{s}$. The corresponding values of the migration energy barriers are in the range 3.46 – 3.89 eV, (iv) in the case of $\text{In}_{0.02}\text{Ga}_{0.98}\text{N}$ alloy, the largest diffusion coefficient possesses a neutral Mg dopant in the local surrounding of 3 In alloy atoms, and the corresponding migration energy barrier is 2.06 eV, (v) the pre-exponential factors of neutral and charged Si dopants are of the order of $0.06 - 0.11 \text{ cm}^2/\text{s}$ and they are accompanied by the migration energy barriers of the order of 3.98 – 4.57 eV.

Effects of Disorder and Stress on AlGa_N multiple Quantum Well Structures studied by Photonic Atom Probe

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Correlative microscopy, combining laser atom probe tomography (La-APT) and photoluminescence (PL), significantly advances the analysis of light-emitting materials such as semiconductors. The photonic atom probe (PAP) exploits the possibility of measuring PL from a specimen during its APT analysis [1], [2], providing a comprehensive understanding of semiconductor materials' characteristics and device performance. In this study, we analyzed a multilayer of AlGa_N/AlN containing 10 quantum wells (QWs), grown by plasma-assisted molecular beam epitaxy, and emitting in the 190–300 nm spectral range [3]. Understanding the correlation between the microscopic characteristics of these heterostructures and their optical properties is crucial for optimizing these structures. The analyzed specimen exhibits spatial inhomogeneities and a significant dispersion of PL emission energy. We show how a correlative microscopy approach can explain different optical emission features of these structures, particularly the distinction between the optical signature of non-defective QWs and QWs lying within the defective regions of this superlattice. For both defective and non-defective quantum wells, the APT compositional maps indicate that transitions most likely stem from wavefunctions localized in quantum dot-like (QD) regions. A striking feature of the set of PL spectra collected is that they exhibit a red shift which evolves dynamically during the PAP analysis. This behavior, already explained for non-polar oxide quantum wells [4], is due to the strain sensitivity of these emitters, acting as local probes for the stress generated by the intense electric field at the sample apex. These results are interpreted through 6-band k.p calculations applied on 1D or 3D models issued from the APT composition maps, and considering the complexity of polar nitride heterostructures. We identify the effect of a field-induced mechanical stress up to around 2 GPa and we are able to connect stress variations to compositional variations and to the variations of the surface electric field, estimated through the abundances of ion species Ga²⁺ and Ga⁺ (charge state ratio).

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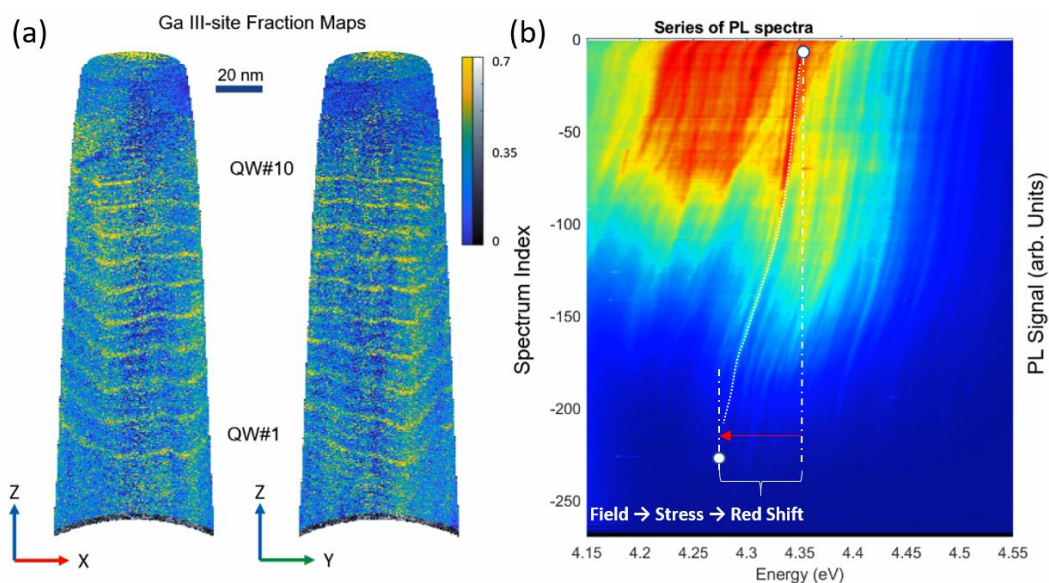


Figure 1 - (a) 2D compositional maps issued from the PAP analysis of an AlGaIn multilayer structure (b) Set of PL spectra acquired in-situ during the APT analysis; the red shift of individual PL peaks is induced by the electric field applied in order to obtain field evaporation

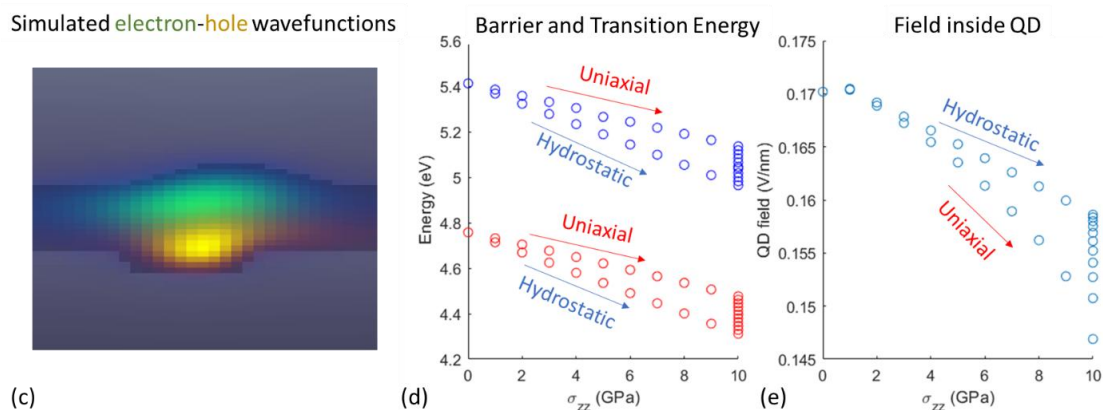


Figure 2 - (c) example of electron-hole wavefunctions calculated in 3D regions mimicking the experimental composition maps; (d) example of calculated dependence of transition energies on applied stress and (e) example of field intensity calculated inside the QD structure.

PEC etching of bulk ammonothermal $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$: defect recognition in a ternary nitride alloy

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Defect-selective photoelectrochemical etching (PEC) is an established technique for revealing crystallographic and electronic inhomogeneities in ammonothermal GaN [1]. This work extends its application to bulk ammonothermal $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$ and systematically compares etching kinetics and defect revelation capability between the two materials.

A difference in PEC etch rate was observed: while n-type ammonothermal GaN required approximately maximum of 30 min to reveal structural inhomogeneities, the $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$ sample required 275 min of cumulative processing — nearly a tenfold increase despite only 6 at.% Al incorporation. This substantial reduction in etch rate is attributed primarily to the wider bandgap and modified photoelectrochemical response of the alloy, and underscores the sensitivity of PEC kinetics to even modest changes in alloy composition.

Despite the slower etch rate, PEC etching successfully revealed growth-related features in AlGa_{0.94}N analogous to those observed in GaN. Growth striations associated with fluctuations in crystallization conditions were clearly resolved, confirming that the PEC mechanism remains sensitive to carrier concentration variations in the ternary alloy [2]. In addition, irregularly shaped regions exhibiting enhanced etch rates became visible after approximately 1 h of processing. Their morphology and orientation versus to the growth interface indicate compositional or doping-related inhomogeneities of growth origin.

Photoetching also revealed hillock-related line features and triangular planar defects. The morphology and etch-rate contrast of these triangular features are consistent with inter-hillock growth region (IHGR) non-homogeneities previously identified in ammonothermal GaN [3], indicating that the same hillock-coalescence-driven crystallization mechanism operates in $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$. This confirms that local growth-rate variations at hillock sidewalls produce extended planar inhomogeneities with distinct electronic properties also in ternary nitride alloys.

Complementary defect-selective etching in molten KOH–NaOH eutectic with MgO (E+M method) was applied to both Ga- and N-polar surfaces of ammonothermal $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$. Threading dislocations were effectively revealed, and the overall dislocation density in studied samples ranged from locally 10^6 cm^{-2} to defect-free areas that covered more than 60% of (0001) sample surface. The etch pit morphology was closely analogous to that in GaN, suggesting that Burgers-vector-dependent dissolution behaviour in the alloy [4].

These results demonstrate that PEC etching, despite significantly reduced etch rate, remains a sensitive and informative technique for defect recognition in bulk ammonothermal AlGa_{0.94}N. The observation that growth striations, IHGR planar inhomogeneities, hillock-related features and threading dislocations are all present and resolvable in $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$ confirms the broader applicability of PEC-based characterization to ternary nitride alloys, and establishes a baseline for defect assessment in ammonothermal AlGa_{0.94}N substrates of increasing technological relevance.

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Acknowledgment

This research was funded by the Polish National Science Center through Project no. 2020/39/D/ST5/01611.

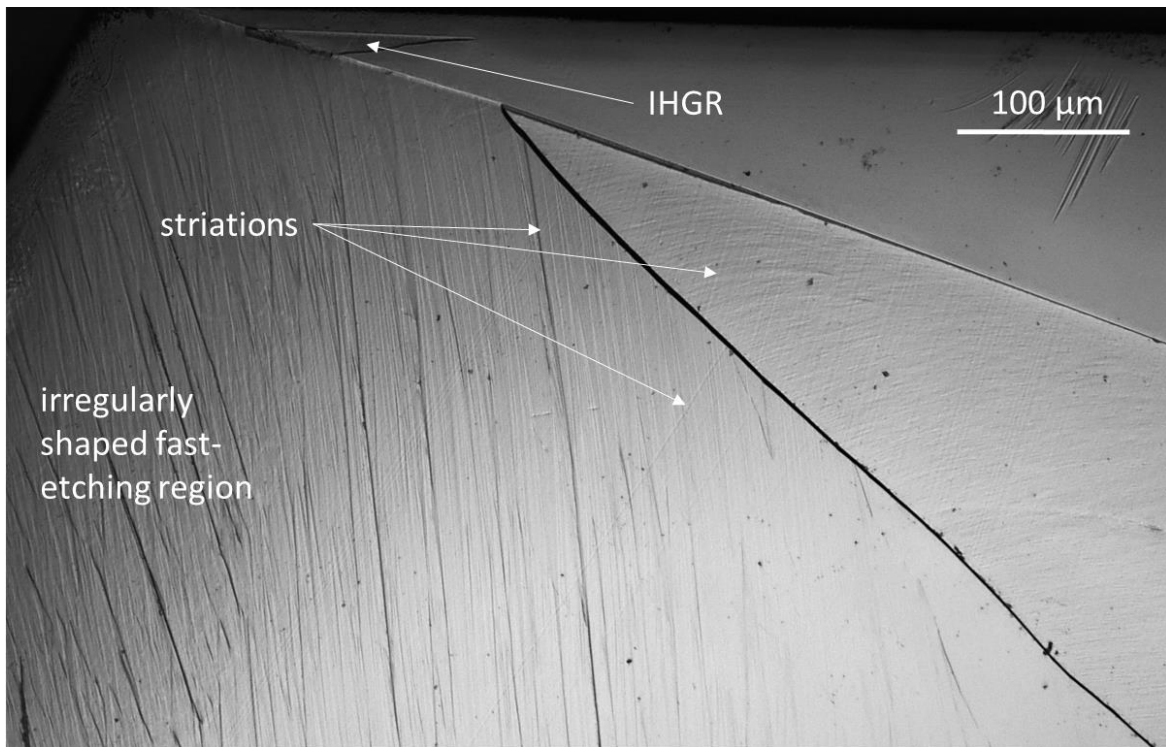


Figure 1. PEC etching results for ammonothermal $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$. (a) Growth striations and irregularly shaped fast-etching regions revealed after ~ 1 h of processing. (b) Hillock-related line features and triangular planar defects (IHGR-type) visible after 275 min cumulative etching.

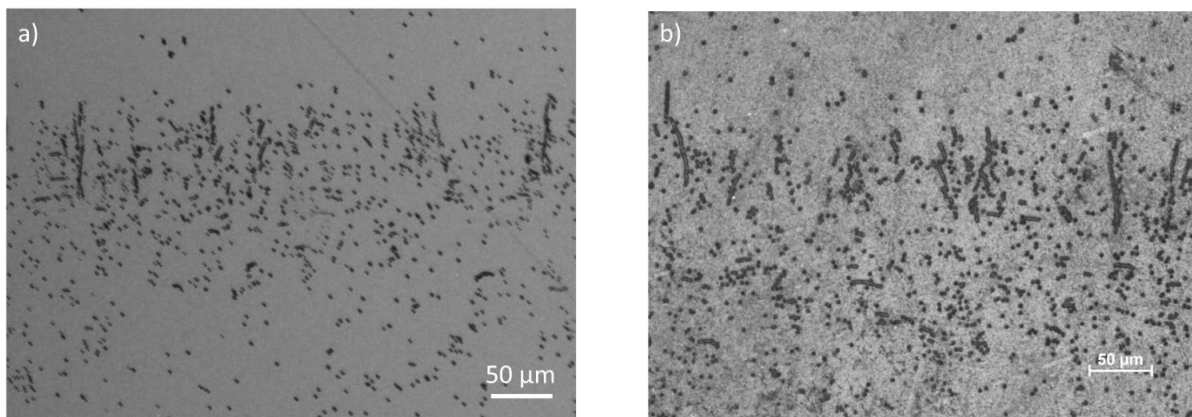


Figure 2. DSE (E+M method) etch pit images on (a) Ga-polar and (b) N-polar surfaces of ammonothermal $\text{Al}_{0.06}\text{Ga}_{0.94}\text{N}$.

Mechanisms of increased luminescence of GaN nanowires covered with HfO_x shells

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Methods for controlling the surface conditions of semiconductor nanowires, especially those made from group III nitrides, and inhibiting their potentially detrimental effects on the transport and optical properties of the system remain an important and current subject of research. Coating nanowires with oxides is considered one of the effective methods for protecting and passivating the sidewalls of GaN nanowires.

In this work, complementary experimental methods providing surface sensitivity or submicrometer spatial resolution were used to understand how coating GaN nanowires with HfO_x leads to a five-fold increase in the maximum cathodoluminescence intensity of this system. The cathodoluminescence spectroscopy and imaging show that, for the GaN nanowires with HfO_x shells, the strongly increased contribution to the near-band-edge luminescence at 3.46 eV has different source than the feature characteristic of bare GaN nanowires, observed at the same energy and ascribed to the exciton decay at inversion-domain boundaries (Fig. 1). The dependence of the cathodoluminescence intensity on the electron beam power indicated that this emission is related to exciton relaxation and not to the emission of structural defects or impurities. X-ray photoelectron spectroscopy enabled us to determine the energy position of the Fermi level pinning at the surface and to exclude a direct influence of the surface band bending, due to HfO_x deposition, on the increase of the luminescence intensity. X-ray absorption spectroscopy revealed nitrogen "pulling" from the near-interface GaN layer during HfO_x deposition.

The analysis of the collected data led to the conclusion that the increase in luminescence of GaN/HfO_x nanowires is related both to the increase in population of O_N centers binding excitons in GaN and the appearance of exciton recombination centers at the interface, emitting luminescence at 4.36 eV, also related to oxygen, as indicated by comparative experiments with Al₂O₃ - an oxide with a different cation. However, in the case of GaN/HfO_x, the increase in luminescence efficiency is achieved at the expense of deterioration of the structural quality of the interface, which manifests itself in the depletion of nitrogen from the sub-interface layer of GaN. An alternative solution for GaN nanowire surface passivation and luminescence efficiency improvement could be the GaN/Al₂O₃ system. In this case, the cathodoluminescence increase is similar, but the XAS results indicate that the sub-interface GaN layer is less modified.

Acknowledgment

This work was partially supported by the Polish NCN grants 2022/45/B/ST5/02876, 2021/43/D/ST7/01936 and 2022/04/Y/ST7/00043 (Weave-UNISONO). This work was also partially developed under the provision of the Polish Ministry and Higher Education project "Support for research and development with the use of research infra-structure of the National Synchrotron Radiation Centre SOLARIS" under contract no 1/SOL/2021/2.

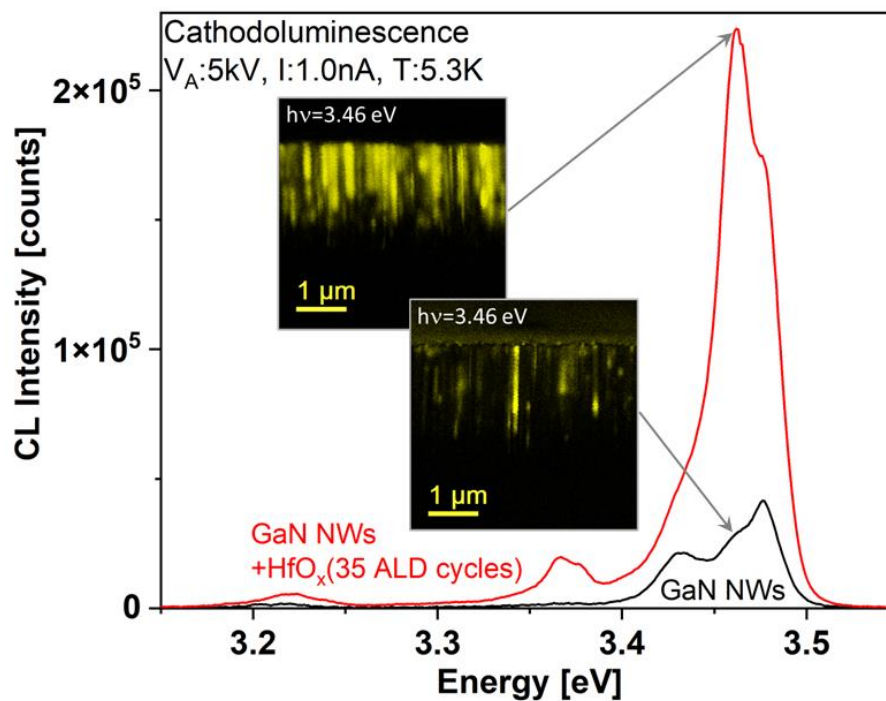


Figure 1: Cathodoluminescence spectra and cathodoluminescence maps acquired for the bare GaN nanowires and the nanowires covered with HfO_x during ALD process lasting 35 cycles. The maps were taken for the photon energy corresponding to the spectral features marked with the arrows.

07

SiC II

TUESDAY · 1 SEPTEMBER 2026

14:30–17:00

Hall of Mirrors

Chair: Carsten Richter

PRESENTATIONS

- 7.0** **Balaji Raghothamachar** INVITED
On the origins of defects and their evolution in bulk and epitaxial 4H-SiC crystals
- 07.1** **Agnieszka Corley-Wiciak**
Correlated Rocking Curve Imaging and Scanning X-ray Microscopy of Dislocations and Interface Strain in Epitaxial 4H-SiC
- 07.2** **Arash Estiri**
Dislocation Type Identification and Classification in 4H-SiC by Synchrotron Rocking Curve X-Ray Diffraction Imaging (RC-XRDI): A Signature-Based Approach
- 07.3** **Zeyu Chen**
Analysis of High Energy Synchrotron X-ray Topography
- 07.4** **Jianpei Zhang**
Analysis of Diffuse X-ray Scattering from Polished SiC wafers by Synchrotron X-ray Topography
- 07.5** **Kaixuan Zhang**
Investigation on the formation of Dislocation Clusters in 4H-SiC Substrate Wafers with Synchrotron X-Ray Topography

On the origins of defects and their evolution in bulk and epitaxial 4H-SiC crystals

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The widespread adoption of silicon carbide (4H) wide bandgap semiconductors for power devices in electric vehicles and chargers, railway, power grid and other high voltage applications requires improved yield during device fabrication. To achieve this, minimizing the densities of crystallographic defects in PVT-grown substrates and CVD-grown epilayers is imperative and this requires an intimate understanding of the processes of generation and nucleation of such defects. A review is presented of the mechanisms of defect replication, propagation, modification, nucleation and multiplication in 4H-SiC PVT grown substrates and CVD-grown homo-epitaxial layers [2]. The replication of Threading Screw and Mixed Dislocations (TSDs and TMDs), Threading Edge Dislocations (TEDs), Stacking Faults (SFs) and Partial Dislocations (PDs) from seeds during PVT growth (Fig.1) [2] and from substrates during CVD [3] will be discussed. The propagation of Basal Plane Dislocations (BPDs) under thermal gradient induced stress on the basal plane will be described as will the propagation of dislocations belonging to the prismatic slip system under the action of stresses originating from a radial thermal gradient [4]. The modification of TMDs and TSDs by macro-step overgrowth leading to the formation of various types of grown-in SF will be explained [5]. The redirection of Basal Plane Dislocations (BPDs) into TEDs during PVT and CVD growth will be clarified as well as the converse redirection of TEDs into BPDs. The nucleation of dislocations at inclusions during PVT-growth will be elucidated. This will include the nucleation of opposite sign pairs of TMDs, TSDs and TEDs as C inclusions; the prismatic punching of dislocation loops at refractory metal inclusions [6], the nucleation of half loops of Basal Plane Dislocation (BPD) at 3C inclusions in homo-epitaxial layers, and the nucleation of half loops of BPD at the epilayer surface. Various mechanisms of creation of low angle grain boundaries (LAGBs) will be described (Fig.3). Multiplication of BPDs in substrates via the Frank-Read mechanism will be explained in detail showing the origins of the pinning points (Fig.2,3) [7,8]. Similarly, the multiplication of PDs during thick epilayer growth will be described [9]. The generation of interfacial dislocation during epilayer growth will also be described as well as the mechanism of formation of Half Loop Arrays during such relaxation processes [10]. Strategies for the mitigation and control of these various mechanisms will be discussed.

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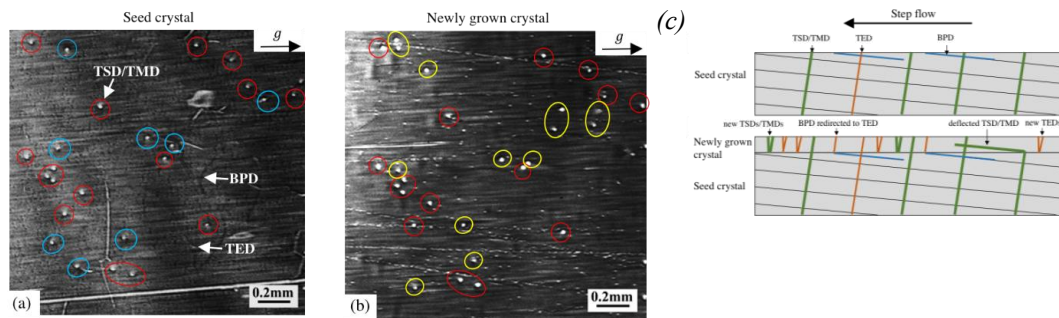


Fig. 1. $11\bar{2}8$ SMBXT images showing dislocation behavior in seed crystal (a) newly grown crystal (b). TSDs/TMDs (red) are replicated to the grown crystal. TSDs/TMDs (blue) get deflected onto basal plane by the step flow of macro-steps. TSDs/TMDs (yellow) are newly generated at the seed/crystal interface. (c) Schematic of dislocation propagation in seed and newly grown crystal [3]

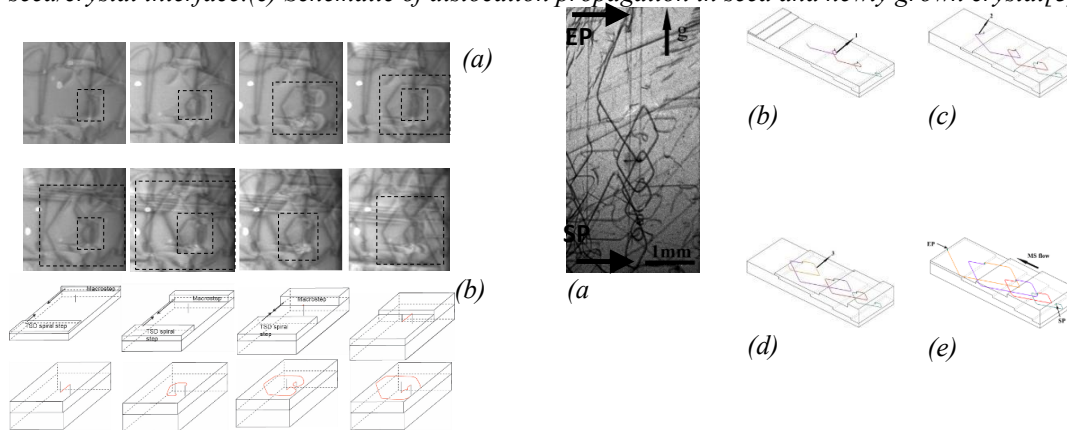


Fig. 2. (a) In situ X-ray topography images illustrating the operation of the double-ended Frank Read Source process during high temperature treatment. (b) Schematic of the deflection of a TED onto the basal plane by a macrostep followed by re-deflection back into threading direction through the encounter between macrostep and TSD spiral advanced in opposite direction during PVT growth. [8]

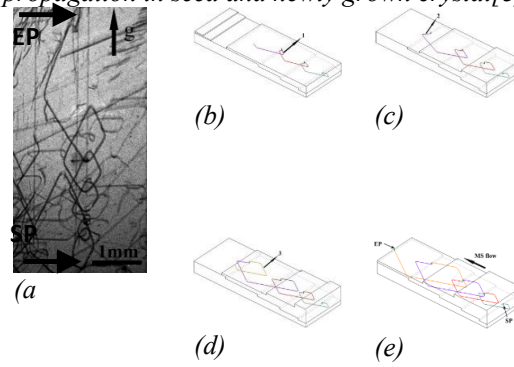


Fig. 3. (a) Transmission X-ray topograph ($g=11\bar{2}0$) showing a diamond shaped BPD loop (SP – starting point; EP – ending point). (b)-(d) Schematic of the formation of a single-ended Frank-Read source through the deflection of a TED into a BPD and back again. [7].

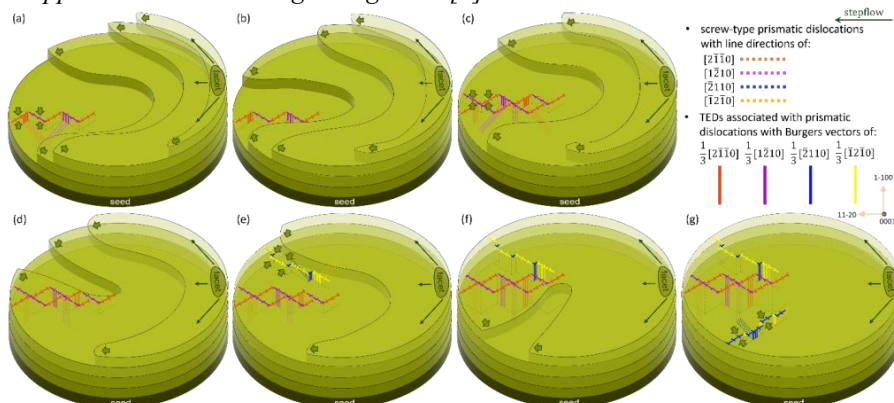


Fig. 4: Schematic diagrams showing the formation mechanism of TED LAGB network through the horseshoe shaped growth steps model [6].

Correlated Rocking Curve Imaging and Scanning X-ray Microscopy of Dislocations and Interface Strain in Epitaxial 4H-SiC

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Silicon carbide (SiC) has become a cornerstone material for next-generation power electronics owing to its wide bandgap, high thermal conductivity, and high critical electric field. Nevertheless, device performance, yield, and long-term reliability remain strongly affected by crystallographic defects originating from bulk growth and substrate processing. Dislocations, stacking faults, basal plane defects, and local lattice distortions may act as recombination centers, leakage pathways, or drivers of device degradation, making their detection and quantification essential for technology optimization. This work presents advanced X-ray-based, non-destructive methodologies for defect characterization in SiC, spanning wafer-scale screening to local, device-relevant analysis.

We investigate dislocation content and interface strain in power-device-grade 4H-SiC substrates and homoepitaxial structures using high-resolution X-ray diffraction imaging. The aim is to establish a quantitative, non-destructive metrology route that links wafer-scale defect mapping with local strain fields relevant to high-power device operation. The material set includes commercial bulk substrates and device-grade epitaxial wafers.

A combination of rocking curve imaging (RCI) and scanning X-ray diffraction microscopy (SXDM) is employed to probe defects across multiple length scales. RCI provides statistically robust information on crystal homogeneity and defect clustering over large areas, while nanofocused SXDM resolves local strain fields and crystallographic distortions associated with individual defects or defect bundles. RCI measurements at multiple energies and reflections enable improved sensitivity to dislocation types and their propagation through the epitaxial layer. From the recorded rocking curves, maps of integrated intensity, full width at half maximum (FWHM), and peak position are derived to visualize dislocations, strain gradients, and wafer bow. Selected regions are subsequently analyzed by SXDM to obtain nanometre-resolved strain information and refine the structural interpretation.

These approaches are fully non-destructive and compatible with intact or partially processed wafers, enabling feedback at multiple stages of the fabrication chain. By linking defect populations and local strain signatures to material quality metrics relevant for power devices, X-ray diffraction microscopy provides a quantitative basis for substrate qualification, process optimization, and reliability-oriented material selection. Such multiscale defect metrology strengthens the understanding of structure–property relationships in SiC and supports the continued development of high-efficiency, high-reliability SiC power technologies.

References

Acknowledgment

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Dislocation Type Identification and Classification in 4H-SiC by Synchrotron Rocking Curve X-Ray Diffraction Imaging (RC-XRDI): A Signature-Based Approach

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Defects in 4H-SiC, including threading screw dislocations (TSDs), edge dislocations (TEDs), mixed dislocations (TMDs), stacking faults (SFs) and particularly basal plane dislocations (BPDs) critically limit device performance and reliability. Conventional rocking-curve X-ray diffraction imaging (RC-XRDI) analysis methods, based on Gaussian fitting, fail to capture the full complexity of non-Gaussian diffraction peak broadening caused by such defects. In this study, by applying the novel cumulative integrated intensity (CII) method [1], schematically shown in figure 1, two metrics are introduced: assumption-free rocking curve integrated intensity (RCII) and Gaussian-based assumption CII slope, to robustly identify and classify defects in 4H-SiC.

Synchrotron RC-XRDI was applied to both 10 μm thick epilayer, denoted by “E”, and bare 4H-SiC, denoted by “B”, wafers diffracting from different crystal planes, all in reflection geometries: (2 2 $\bar{4}$ 16) at 17.48 keV, (1 1 $\bar{2}$ 8), (1 $\bar{1}$ 0 7), and (0 0 0 8) at 9.0 keV. Synchrotron RC-XRDI integrated intensity images are presented in figures 2 and 3.

Spearman correlation analysis confirms the claims of Khaliq *et al.*, [2] that defects reduce RCII and increase peak broadening. These two effects collectively decrease the CII slope. RCII also directly correlates with maximum intensity of rocking curve, so reduced RCII lowers the maximum intensity of rocking curve. Generally, maximum intensity and full width at 1% of maximum intensity (FW1%M) and full width half maximum (FWHM) are inversely correlated. Exceptionally for regions affected by TEDs, maximum intensity and FW1%M show a direct correlation. In the full paper, the effects of each defect on relative peak position (RPP, subtraction of defect peak position from the matrix peak position) and on peak broadening across each reflection are discussed in detail.

Our results show that different defect types exhibit different RC-XRDI signatures that cannot be resolved using conventional metrics such as FWHM and RPP, presented in figures 4 and 5. The primary limitation arises from the substantial overlap between these parameters for different defect classes, which obscures their individual characteristics and prevents unambiguous identification. In contrast, the newly developed metrics successfully reveal these characteristics, enabling identification and classification of defects, as shown in the histograms of CII slope depicted in figures 6 and 7. While BPDs are a distinct class of defect from the threading dislocations (TDs), this novel approach differentiates TMDs and TSDs (which KOH etch cannot do) [3], discriminates different defects from the matrix, and reveals the intrinsic TED-like or TSD-like characteristics of BPDs.

These two metrics offer a framework for a non-destructive classification of defect types in 4H-SiC, outperforming traditional FWHM- and peak position metrics, providing a compelling

alternative to KOH etching, and supporting improved wafer qualification, device performance, and long-term reliability

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Acknowledgment

We acknowledge the Diamond Light Source (DLS) for beamtime under proposal MM28722 and OM40233-1. A. Estiri is a PhD student, part funded by DLS and Bruker Ltd. The study is supported by funding from EPSRC through grant numbers EP/P017363/1 and EP/W.

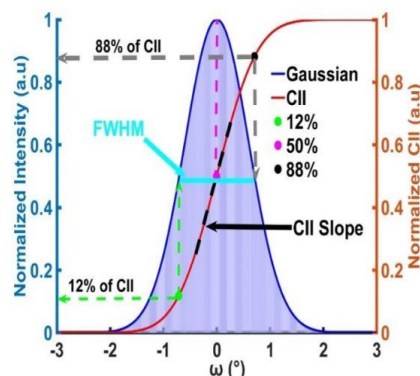


Figure 1. Correlation between the CII and an ideal Gaussian curve. 50% of CII represents the peak position of a Gaussian curve, while 12% and 88% are the lower and upper bounds of the FWHM [1].

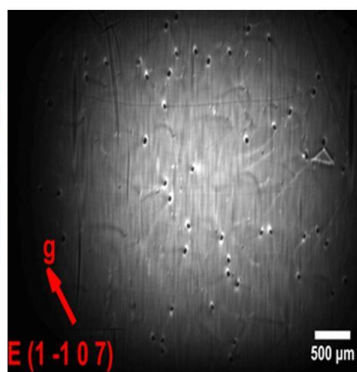


Figure 2. Synchrotron RC-XRDI. Integrated intensity image collected at 9.0 keV

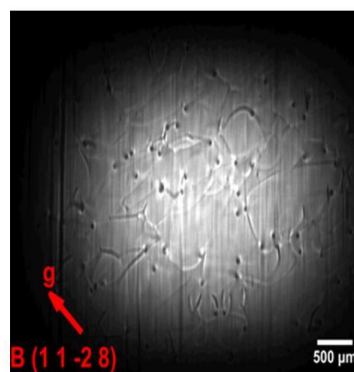


Figure 3. Synchrotron RC-XRDI. Integrated intensity image collected at 9.0 keV

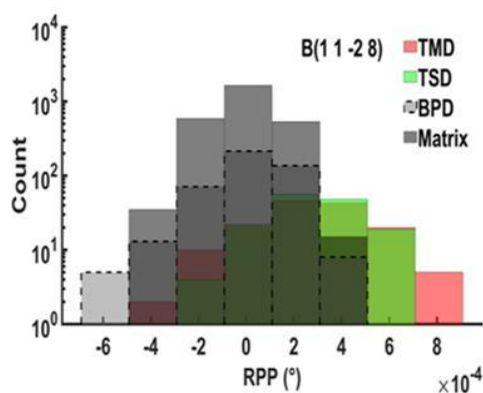


Figure 4. Histogram of RPP for B(1 1 -2 8).

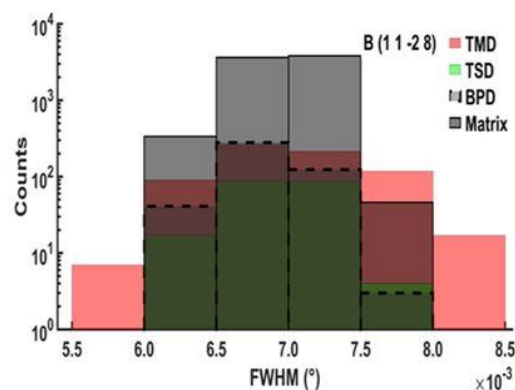


Figure 5. Histogram of FWHM for B(1 1 -2 8).

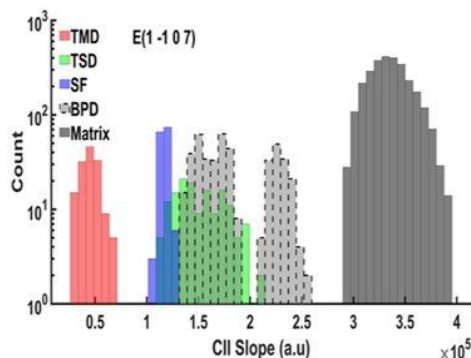


Figure 6. Histogram of CII slope for E(1 -1 0 7).

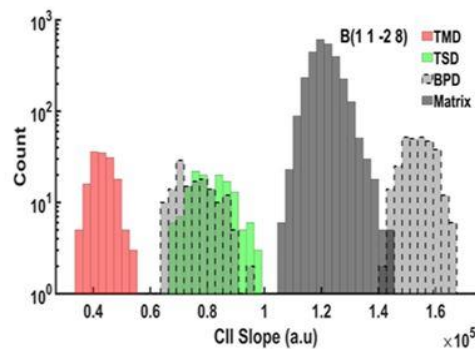


Figure 7. Histogram of CII slope for E(1 1 -2 8).

Analysis of High Energy Synchrotron X-ray Topography

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Silicon carbide (SiC) is a wide bandgap semiconductor that has been extensively used in power electronics due to its superior properties, including a wide bandgap, high breakdown voltage, and excellent thermal stability. However, crystal defects such as TEDs, TSDs, and BPDs can significantly degrade device performance [1,2], making their characterization essential for improving the quality of 4H-SiC wafers. Synchrotron monochromatic beam X-ray topography (SMBXT) is a powerful technique for defect characterization, offering a large field of view and high-contrast imaging of defects. While SMBXT using the 11-28 reflection has been widely adopted, its penetration depth (approximately 17 μm [3]) is insufficient for analyzing devices with deep PN junctions. Consequently, there is a need for alternative reflections that provide both greater X-ray penetration and clear defect contrast.

High energy SMBXT can be used to achieve great penetration depth, where the 22-4 16 reflection, a harmonic of 11-28, offers improved defect contrast, higher strain sensitivity, and increased penetration depth (around 30 μm), making it a promising candidate for advanced characterization [4]. In addition to greater penetration depth, high energy X-ray topography can also provide higher sensitivity to lattice distortion. Synchrotron white beam X-ray topography (SWBXT) in transmission geometry in 3-300 reflection have been carried out in 27-ID (HEX) beamline of National Synchrotron Light Source II in Brookhaven National Laboratory. Fig.1 shows enlarged topograph of 3-300 reflection of 4H-SiC with 12 μm epilayer. Contrasts of BPDs in 3-300 reflection (Fig. 1(b)) behave differently from 1-100 reflection (Fig. 1(a)), where bimodal contrast can be observed since the X-ray is more sensitive to the strain field around the core of dislocation[5]. In this paper, formation of bimodal contrast will be analyzed.

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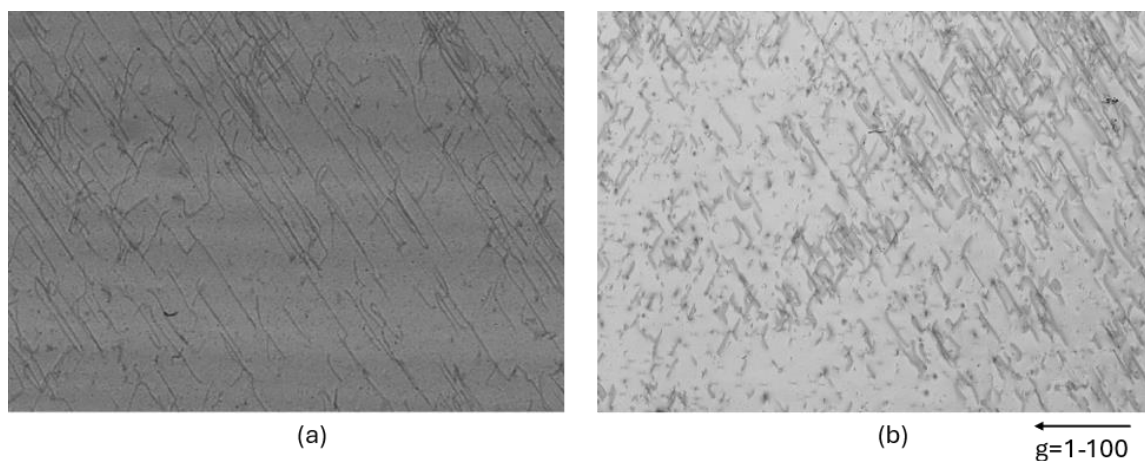


Figure 1: enlarged topograph of 4H-SiC epiwafer (a) in 1-100 reflection and (b) in 3-300 reflection.

Analysis of Diffuse X-ray Scattering from Polished SiC wafers by Synchrotron X-ray Topography

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Silicon carbide (SiC) is a key semiconductor material for next-generation electronics, microelectromechanical systems, and high-power, high-temperature applications. Its advantages include a wide bandgap, high carrier mobility, excellent thermal conductivity, and outstanding mechanical strength[1]. SiC substrates must have a damage-free surface for the growth of high-quality epilayers for device fabrication[2], [3]. Surface preparation processes such as sawing, and mechanical polishing inevitably damage surface and subsurface atomic layers and wafer handling can introduce surface damage likes scratches[4], [5]. Such surface damage can be assessed using X-ray diffraction by analyzing the diffuse scattering. Diffuse scattering is the weak continuous scattering that occurs between the Bragg reflections and arises from crystal disorder, i.e., deviations from an ideal periodic atomic arrangement. Diffuse scattering can be measured by high resolution X-ray diffraction methods but whole wafer mapping can be time consuming[6]. Synchrotron X-ray topography is a diffraction-based, non-destructive imaging technique that utilizes the high brightness, tunability, and natural collimation of synchrotron radiation to visualize defects in single crystals. Based on Bragg diffraction, local lattice distortions caused by defects modify the diffracted intensity and generate contrast in the image. Owing to its strong sensitivity to lattice distortion, it has been widely used for evaluating crystal quality and detecting structural damage in both industry and research[7], [8]. In this work, we investigated diffuse X-ray scattering associated with polishing-induced scratches in SiC wafer with synchrotron X-ray topography technique for the first time. Figure 1. (a) shows the grazing image on (11-28) reflection of SiC wafer and the center gray contrast region induced by polishing scratches is outlined with yellow line. The selected regions for scratch comparison are labeled in red. Figure 1. (b)–(c) are high-magnification images of these regions. The scratches are marked with green lines, and the boundaries between the center gray contrast region and the normal region are indicated by yellow lines. The density of scratches in the gray center region is much higher than from other regions. The usefulness of the diffuse scattering data from X-ray topography is assessed by comparison with X-ray diffraction measurements from these wafers.

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Acknowledgment

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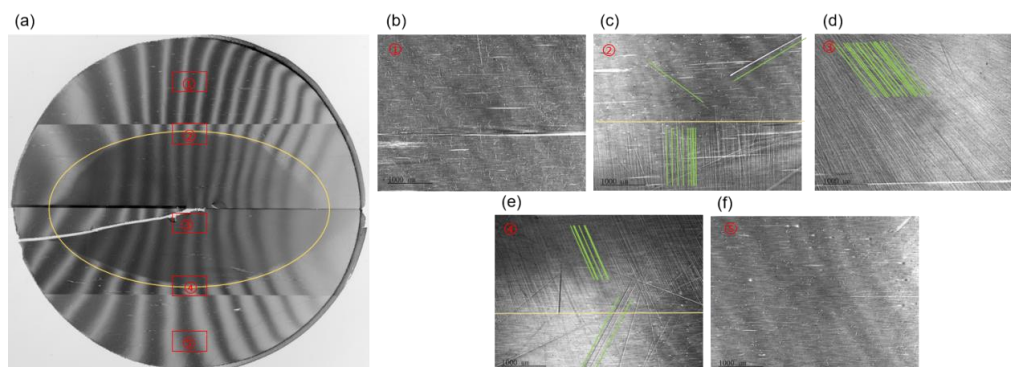


Figure 1. (a) The central gray contrast region induced by polishing scratches is outlined with yellow lines in the (11-28) grazing image. The selected regions for scratch comparison are labeled in red. (b)–(f) High-magnification images of these regions. The scratches are marked with green lines, and the boundaries between the black contrast region and the normal region are indicated by yellow lines.

Investigation on the formation of Dislocation Clusters in 4H-SiC Substrate Wafers with Synchrotron X-Ray Topography

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Silicon Carbide (SiC) has emerged as a premier wide-bandgap semiconductor, garnering significant attention due to its exceptional physical properties, most notably its high thermal conductivity, superior electron saturation velocity, and robust breakdown electric field. These characteristics make SiC an ideal candidate for the next generation of high-frequency and high-power electronics, outperforming traditional silicon in demanding environments like electric vehicle powertrains and 5G communication infrastructure [1, 2]. Despite these advantages, the commercial maturation of SiC technology is currently limited by material vulnerabilities. Specifically, various structural defects within both the substrate and the epitaxial layers can degrade device reliability and electrical performance. Consequently, a comprehensive characterization of these defects and a deeper insight into their formation mechanisms are vital for refining crystal growth processes, enhancing device longevity, and increasing industrial production yields [3, 4].

Two new interesting arrangements of defects in 4H-SiC wafers are discovered and investigated with Synchrotron X-ray Topography in this study. Figure 1 and Figure 2 show the topograph images of these defect arrangements and an illustration of the proposed formation mechanism of these types of defects. One type is the “galaxy” defect arrangement, which was found to be composed of micro-level inclusions, and was proposed to be caused by inclusions from furnace fallouts, the induced threading dislocations, and the pile-up of prismatic slip dislocations and BPDs against the inclusions. The other new arrangement is observed to contain a high-density region of BPDs bounded by two arrays of TEDs. It’s proposed to be formed by cross-slipping of anti-parallel prismatic slip bands. Both of these defect arrangements contain both threading dislocations and BPDs. The investigation of the formation of these defect arrangements provides critical verification of the previous theories on the interaction between different types of dislocations [5].

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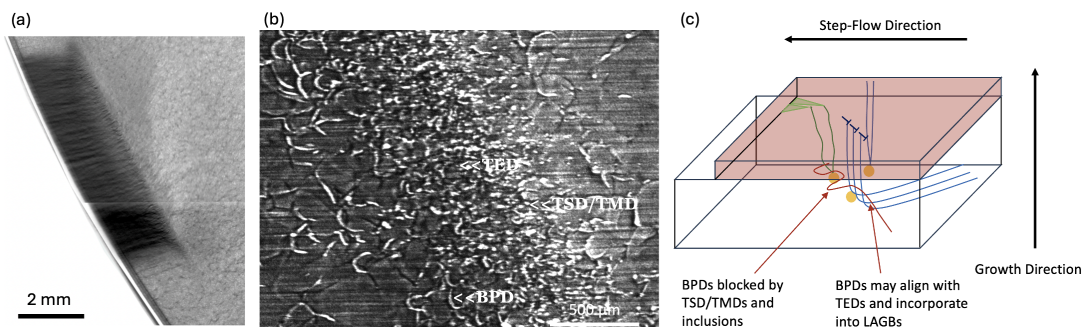


Figure 1: (a) Transmission (1-100) X-Ray topograph image, (b) grazing (11-28) X-ray topograph image, and (c) proposed model for the formation of the "galaxy" defect.

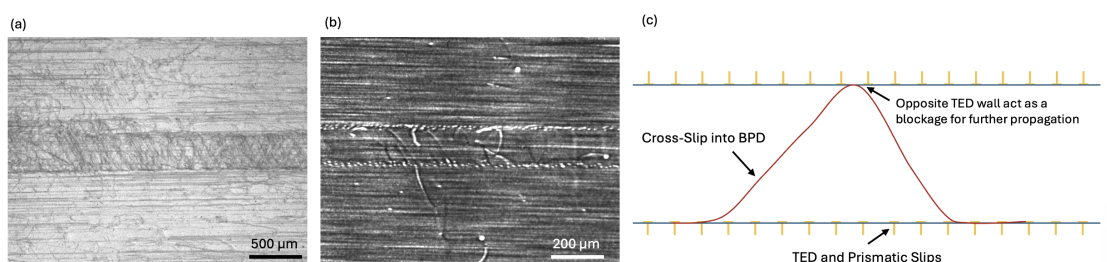


Figure 2: (a) Transmission (11-20) X-Ray topograph image, (b) grazing (11-28) X-ray topograph image, and (c) proposed model for the formation of the newly observed prismatic slip-BPD interaction.

08

Emerging materials

WEDNESDAY · 2 SEPTEMBER 2026

08:50–10:30

Hall of Mirrors

Chair: Filip Tuomisto

PRESENTATIONS

- 8.0** **Anna Kaleta** INVITED
From Heteroepitaxy to Functionality: Transmission Electron Microscopy of NbN-Integrated Nitride Devices
- 08.1** **Janusz Sadowski**
Structural defects in wurtzite MnTe grown by molecular beam epitaxy
- 08.2** **Shiv Singh**
Defect engineering in Sm-based oxypnictide superconducting bulks synthesized via high-pressure techniques
- 08.3** **Lorenzo Rigutti**
Correlative Electron Microscopy and Atom Probe Analysis of ZnS:Cu: Insight in Light Emission Mechanisms

From Heteroepitaxy to Functionality: Transmission Electron Microscopy of NbN-Integrated Nitride Devices

A. Kaleta^{1,2,*}, M. Morales², M.-P. Chauvat², S. Kret¹, P. Dłużewski¹, H. Rotella³,
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Niobium nitride (NbN) integrated with III-nitride (III-N) heterostructures is an emerging material platform for next-generation high-power and high-frequency electronic devices. NbN/III-N hybrid systems enable new device concepts that combine metallic or superconducting functionality with wide-bandgap semiconductor technology, including advanced architectures such as metal-base transistors.

In this work, we investigate the growth and structural properties of III-N/NbN/III-N heterostructures fabricated by ammonia-assisted molecular beam epitaxy (NH₃-MBE) which enables precise control of composition and growth conditions leading to the formation of high-quality crystalline NbN layers epitaxially integrated with III-N materials. The study focuses on three NbN phases—cubic δ -NbN and hexagonal β -Nb₂N and ϵ -NbN—and their controlled phase transformations ($\delta \rightarrow \beta \rightarrow \epsilon$).

A systematic transmission electron microscopy (TEM) study, including diffraction and high-resolution TEM, is used to determine the crystal structures of the NbN phases and their epitaxial relationships with the surrounding III-N layers. Particular attention is given to crystalline quality, structural defects, their potential impact on the physical properties and reliability of future devices. Structural analysis reveals a previously unreported trigonal symmetry phase originating from ordered nitrogen vacancies within the hexagonal β -Nb₂N structure (Figure 1). Furthermore, we investigate unexpected polarity reversal in III-N layers epitaxially grown on NbN, which opens new opportunities for the fabrication of nitrogen polar devices.

By correlating atomically resolved TEM analysis with the phase composition of NbN, this work establishes structure–property relationships relevant to device performance and reliability in NbN-integrated III-nitride electronics.

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Acknowledgment

This work has been financially supported with NIOBIUM project (No. ANR-21-CE08-007), POLONIUM NAWA (BPN/BFR/2023/1/00021/U/00001)

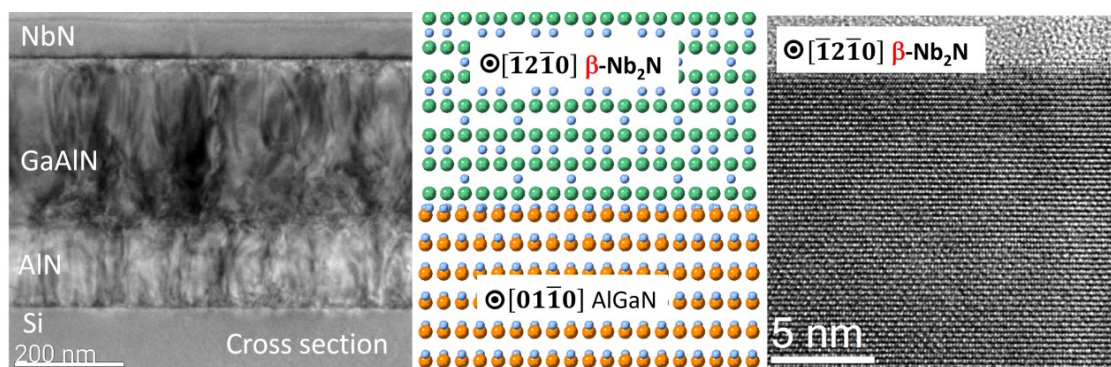


Figure 1. TEM investigation of the Si/AlN/GaAlN/NbN heterostructure (left) reveals the presence of β -Nb₂N with a previously unreported trigonal symmetry, illustrated by the ball-and-stick model (middle). High-resolution TEM (HRTEM) image of the β -Nb₂N phase (right), recorded along the same crystallographic projection as the structural model.

Structural defects in wurtzite MnTe grown by molecular beam epitaxy

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MnTe belongs to the newly identified altermagnetic materials. Akin to antiferromagnets altermagnets have fully compensated magnetic moment, but their electronic bands are spin-polarised. Because of that and also due to high Néel temperatures, the altermagnetic materials attract a lot of attention as candidates for perspective applications in spintronic devices.

MnTe can occur in several crystalline polytypes: α , β , γ and δ phases ascribed to hexagonal NiAs type (nickeline), hexagonal wurtzite, cubic zinc blende and cubic rock-salt structure, respectively. In normal conditions hexagonal α is a typical crystallographic structure of MnTe, and in this polytype MnTe is considered as a canonical (g-wave) altermagnet.

Zinc-blende γ -MnTe phase occurs only in epitaxial layers grown on suitable substrates. Rock-salt structure (δ phase) is metastable and can be stabilized e.g. by pressure; whereas wurtzite (wz) β -MnTe to our knowledge has been reported so far only in nonhomogeneous MnTe thin films as small admixture of secondary crystalline phase regions.

Using molecular beam epitaxy (MBE) technique we have succeeded in growing thin monocrystalline layers of scarcely studied wurtzite β -MnTe as epitaxial layers deposited directly on GaAs(111) substrates. By slight variations of the growth conditions we can obtain: (i) pure wz β -MnTe, (ii) pure nickeline α -MnTe, (iii) mixture of these two polytypes (see Fig.1). In each case different structural defects have been identified: mostly stacking faults and inclusions of zinc-blende γ -MnTe phase. As for the altermagnetic properties of β -MnTe, there is no consensus, yet to our knowledge. By analogy to altermagnetic wurtzite MnSe it cannot be excluded, [4] but there is no definite proof for that yet, neither from theory nor from experiment.

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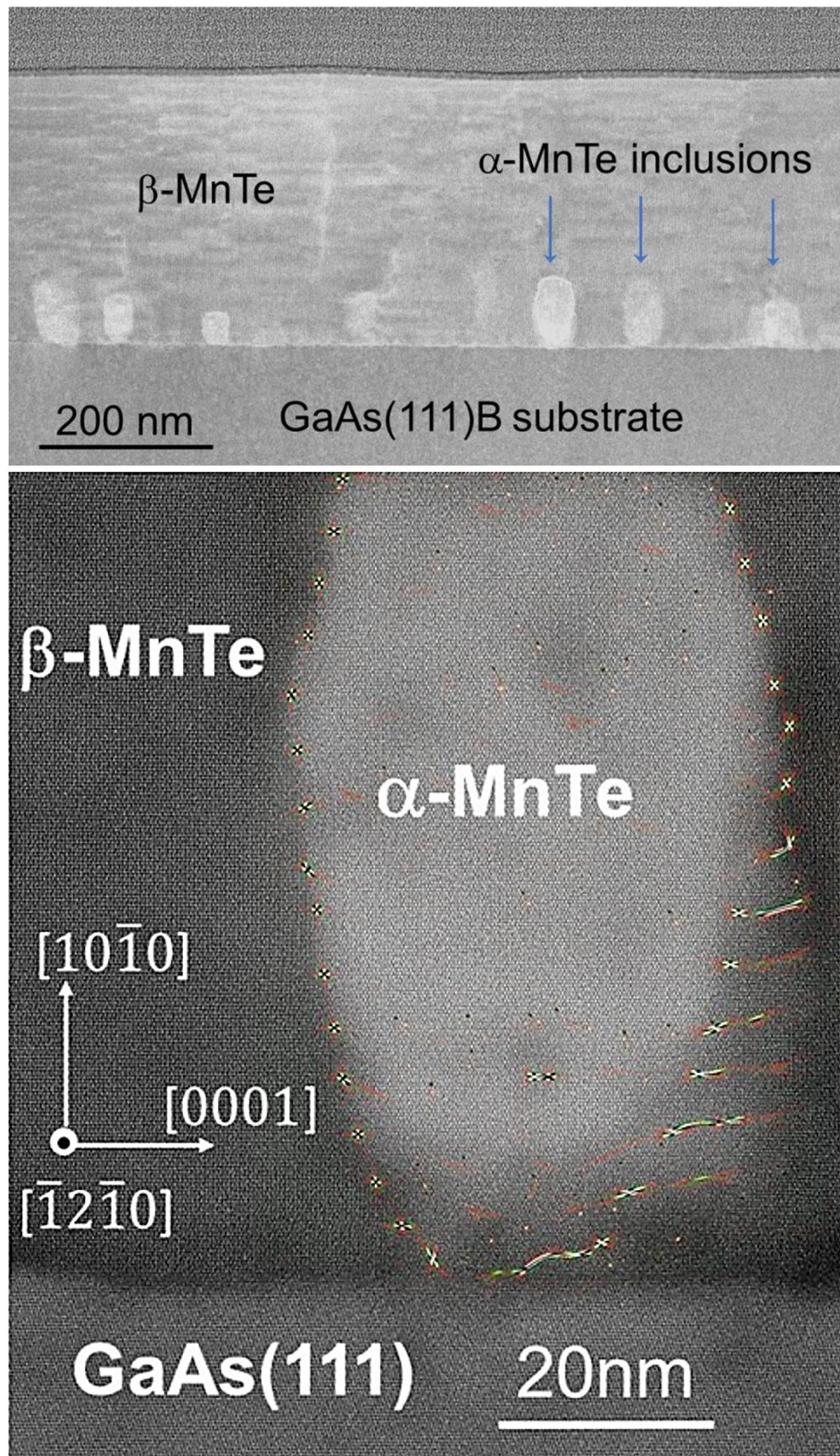


Figure 1: Cross-sectional TEM images of wurtzite β -MnTe layer grown by MBE on GaAs(111)B substrate. Inclusions of nickeline α -MnTe are located at the GaAs-MnTe interface region .

Defect engineering in Sm-based oxypnictide superconducting bulks synthesized via high-pressure techniques

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Defect engineering plays a pivotal role in tuning the physical properties of iron-based superconductors, where controlled defect structures can significantly enhance superconducting performance. In this work, we systematically investigate the influence of synthesis conditions on defect formation and superconducting properties of F-doped SmFeAsO_{0.8}F_{0.2} (Sm1111) bulk samples prepared using various high-pressure (HP) techniques, including high gas pressure–high temperature synthesis (HP-HTS), cubic-anvil high-pressure (CA-HP), and spark plasma sintering (SPS), in comparison with conventional solid-state synthesis at ambient pressure (CSP-AP). The applied synthesis routes, involving pressures up to 4 GPa and temperatures up to 1600 °C, enable precise control over phase formation, defect density, and microstructural homogeneity. Our results demonstrate that HP conditions strongly affect the generation and distribution of defects such as vacancies, grain boundaries, and compositional inhomogeneities, which directly influence key superconducting parameters. Optimized high-pressure synthesis significantly improves grain connectivity, reduces porosity, and enhances phase purity, leading to higher critical current density and stronger flux pinning, while maintaining or slightly improving the superconducting transition temperature (T_c). In particular, *in-situ* synthesis requires higher pressure and temperature (4 GPa, 1400 °C, 1 h) to achieve the complete phase formation and introduces beneficial defects that increase T_c by approximately 3 K. In contrast, *ex-situ* synthesis can be performed at much lower pressure (0.5 GPa), where grain-boundary defect engineering results in an order-of-magnitude enhancement in critical current density while preserving T_c (~53 K). These findings demonstrate that controlled defect engineering via high-pressure synthesis is an effective strategy for optimizing the performance of Sm-based oxypnictide superconductors and advancing the design of high-performance superconducting materials.

References

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Acknowledgment

This research was supported by the National Science Centre (NCN), Poland through the SONATA-BIS 11 project (2021/42/E/ST5/00262) and the Weave-UNISONO project (2025/07/Y/ST5/00116). SJS acknowledges financial support from NCN Poland through Project numbers 2021/42/E/ST5/00262 and 2025/07/Y/ST5/00116.

Correlative Electron Microscopy and Atom Probe Analysis of ZnS:Cu: Insight in Light Emission Mechanisms

Roberto Hernandez¹, Lorenzo Rigutti², Jonathan Houard², Ludovic Largeau¹, Stefano Pirotta¹,
Nathaniel Findling¹, Francois Julien¹, Jules Duraz¹, Maria Tchernycheva¹

¹Centre de Nanosciences et de Nanotechnologies (C2N), Univ. Paris-Saclay, 91120 Palaiseau, France

²UNIROUEN, CNRS, Groupe de Physique des Matériaux, Normandie Université, 76000 Rouen, France

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ZnS:Cu powders are experiencing renewed interest as a primary candidate for light emitters based on Alternating Current Electroluminescence (ACEL) technology, enabling large-area, cost-effective, deformable light sources. Yet, the understanding of fundamental light emission mechanism – still a matter of debate [1] – may be significantly improved by atomic scale, correlative microscopy analysis. Traditional models attribute this to Cu₂S precipitates facilitating carrier injection, whereas more recent works suggest copper segregation at structural defects [2]. Historically, these features remained unvalidated due to the low sensitivity of conventional detection methods. Furthermore, while stacking faults are recognized as a prerequisite for emission [3], the physical basis for this requirement remains elusive.

ZnS:Cu grains exhibit emission characteristics with a broad-band EL emission (2.15-3.15 eV). This was evidenced by either placing the grains directly on top of interdigitated electrodes or by fabricating fully processed films. A comparative analysis using cathodoluminescence (CL) and photoluminescence (PL) highlights a clear divergence in excitation pathways: unlike PL and CL, the EL emission is strictly governed by the internal structural defects evidenced through nanoscale analysis.

This was achieved through the application of correlative Atom Probe Tomography (APT) and Transmission Electron Microscopy (TEM). The internal lattice defects revealed by etching, specifically triangular etch pits and surface striations, served as structural indicators, as the pit apices align with the c-axis in hexagonal (wurtzite) and one of the four [111] axis in cubic (sphalerite) structure. These crystallographic benchmarks guided the Focused Ion Beam (FIB) milling, enabling the site-specific preparation of TEM and APT specimens to properly image and digitally reconstruct the ZB-WZ superlattices that TEM could image (Fig. 1). APT unveiled a random Cu distribution with a concentration $n_{\text{Cu}}=3 \times 10^{19} \text{ cm}^{-3}$ throughout the ZnS lattice and even allowed imaging Zincblende-Wurtzite (ZB-WZ) superlattices as a density modulation of detected ions, most likely driven by field-effect mechanisms the fundamental prerequisite for electroluminescence (Fig. 2).

These results call for a revision of established theories and elucidate the functional role of structural defects, features typically regarded as detrimental in semiconductor physics, yet here identified as key facilitators of luminescence. We propose therefore a novel electroluminescence mechanism governed by the unique electronic environment of ZnS:Cu. We present how the alternating ZB-WZ phases allow the appearance of built-in electric fields arising from the spontaneous polarization in the hexagonal phase, and the band gap offset between ZB-ZnS and WZ-ZnS, that facilitate carrier radiative recombination over Cu-related deep levels.

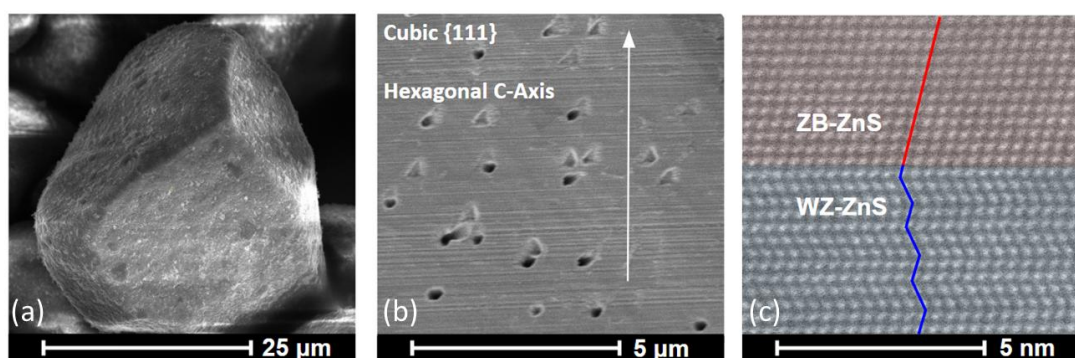


Fig. 1. Structural and interfacial analysis of ZnS:Cu grain. (a) SEM image of a single ZnS particle. (b) SEM image of a grain surface after hydrofluoric acid etching showing surface striations and triangular etch pits that align with the c-axis in hexagonal (wurtzite) and one of the four [111] axis in cubic (sphalerite) structure. (c) TEM image of a Zincblende-Wurtzite superlattice.

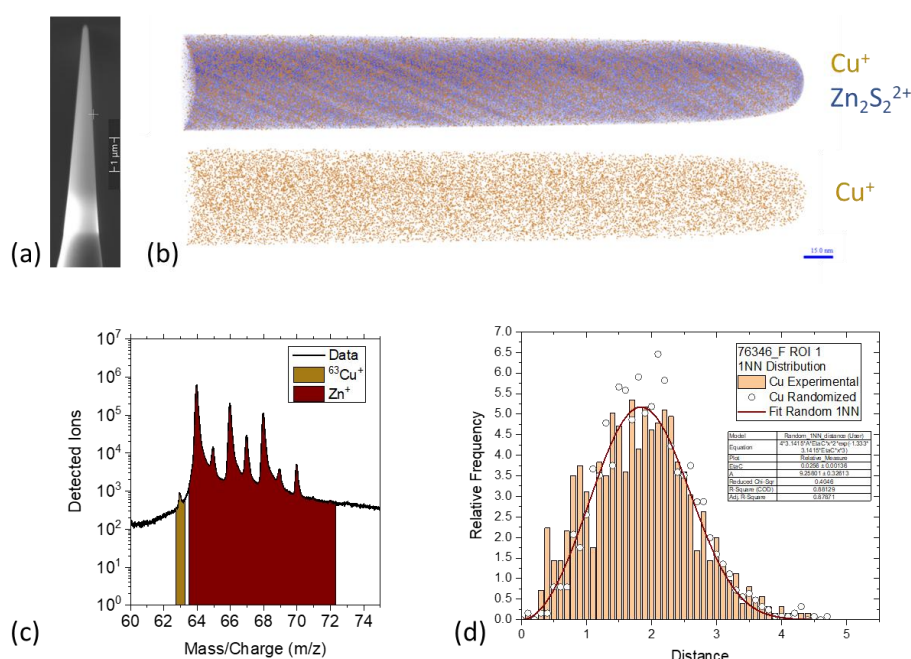


Fig. 2: APT analysis of ZnS:Cu. (a) FIB-prepared field emission tip specimen; (b) 3D reconstructed volume showing the superimposed distribution of Cu^+ atomic ions and $\text{Zn}_2\text{S}_2^{2+}$ molecular ions; (c) detail of the mass spectrum showing the peaks of Cu^+ and Zn^+ ; (d) 1st nearest Neighbor distribution analysis comparing the experimental Cu distribution (bars) with the Cu randomized distribution (circles) and the analytical distribution typical of random solutes.

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09

Modelling

WEDNESDAY · 2 SEPTEMBER 2026

11:00–13:00

Hall of Mirrors

Chair: Daniel Prochowicz

PRESENTATIONS

- 9.0** **José Coutinho** INVITED
Modelling of nitrogen displacements in GaN using first-principles methods combined with junction spectroscopy
- 09.1** **Marta Chabowska**
Defect-Driven Symmetry Breaking in Nanopillar Formation
- 09.2** **Magdalena Załuska-Kotur**
Modelling Defect-Induced Pattern Formation in Discrete Systems
- 09.3** **Dilip Gersappe**
Multiscale Modelling of Stress-Driven Dislocation Formation in SiC Crystal Growth
- 09.4** **Christian Gobert**
Point Emitter Quantification in Photoluminescence Scans using a Convolutional Neural Network

Modeling of nitrogen displacements in GaN using first-principles methods combined with junction spectroscopy

José Coutinho^{1,*}, Christopher A. Dawe², Vladimir P. Markevich², Piotr Kruszewski³, Pawel Prystawko³, Sylwester Bulka⁴, Matthew P. Halsall², Anthony R. Peaker²

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Gallium nitride (GaN) is wide-bandgap semiconductor with remarkable properties for supporting advanced electronic and optoelectronic technologies. Its high breakdown electric field, superior electron saturation velocity and excellent thermal and chemical stability, enable efficient operation under high voltage, high frequency, and high temperature conditions. Combined with its direct bandgap of nearly 3.5 eV, high electron mobility ($2000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$), and outstanding radiation resistance, GaN offers a unique and versatile platform for applications ranging from power conversion to high-speed switching [1].

The presence of defects, either native or extrinsic, can lead to several changes in the electrical, optical or magnetic properties of semiconductors. These can be benign like dopants that control the electrical conductivity, or detrimental, such as grown-in dislocations that profoundly affect carrier scattering and lifetime. It is therefore imperative to understand the underlying properties of these structures, particularly how they respond to device processing treatments and how they interact with external fields and charge carriers.

EE1 and EE2 are among the most conspicuous defect signatures detected by deep level transient spectroscopy (DLTS) after subjecting GaN to electron irradiation [2]. They are responsible for electron traps at about $E_c - 0.2 \text{ eV}$ and $E_c - 1.0 \text{ eV}$, respectively, and can be created when the electron beam energy is well below the $\sim 480 \text{ keV}$ threshold needed for displacing Ga atoms. This observation, along with the nearly linear scaling between the EE1/EE2 DLTS peak intensities and irradiation dose, are strong indications that EE1 and EE2 are defects related to nitrogen displacements [2]. We recently applied DLTS to electron irradiated GaN epi layers grown on top of Ammono-GaN substrates, with electron beam energies below 370 keV [3]. From analysis of the unusual trap filling kinetics and electric field dependence of DLTS peak shape and emission rate, we postulated that EE1 comprises a convolution of signals arising from donor transitions of nitrogen vacancies (V_N) influenced by the electric field of nearby charged nitrogen interstitials (N_i).

We now present the modeling part of this work, which, together with the junction-spectroscopy measurements, guided the development of the final model. We performed a series of first-principles calculations based on hybrid density functional theory, where several defects were inserted in large GaN supercells with up to 300 atoms. Among the estimated properties we present defect stability, transition levels, capture cross sections, defect migration and Frenkel-Pair formation/dissociation mechanisms. The calculations find that an isolated V_N defect introduces a single donor transition in the upper half of the gap at $E_c - E(0/+) = 0.12 \text{ eV}$. We also predict an acceptor level for N_i at $E_c - E(-/0) = 0.71 \text{ eV}$. From inspection of the one-electron band structure we conclude that V_N - N_i complexes form donor-acceptor pairs ($V_N^+ \cdot N_i^-$ in the neutral charge state) with a deep $V_N^+ \cdot N_i^{(-/0)}$ transition level around $E_c - 0.8 \text{ eV}$ involving a trap localized on N_i , and a shallower $V_N^{(0/+)} \cdot N_i^-$ transition level at about $E_c - 0.1 \text{ eV}$ localized on the vacancy.

From a comparison of isolated defect results and combined V_N - N_i pair calculations, we find that the negatively charged N_i^- component in the Frenkel-Pairs repel electrons trapped at nearby vacancies. This effectively raises the energy of neutral V_N^0 units and decreases their $V_N^{(0/+)}-N_i^-$ transition energy with respect to that for isolated V_N . Conversely, the N_i acceptor state is stabilized by the attractive field of a close V_N^+ defect, thus shifting the $V_N^+-N_i^{(-/0)}$ transition deeper within the gap when compared to that for isolated N_i . This behavior not only explains the measured enhancement of the electron emission from $V_N^0-N_i^-$ for those pairs where N_i^- is closest to the filled vacancy trap, but also accounts nicely for observed strong increase of the capture rate involving transitions of remote pairs and isolated vacancies that are free from the electronic screening of N_i^- .

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Acknowledgment

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Defect-Driven Symmetry Breaking in Nanopillar Formation

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The surface morphology and evolution of materials are crucial for the fabrication of electronic and optoelectronic devices. Consequently, the nanoscale morphology of materials – particularly the mechanisms by which it develops through the attachment and reorganization of surface deposits composed of atoms or molecules – remains an active area of research.

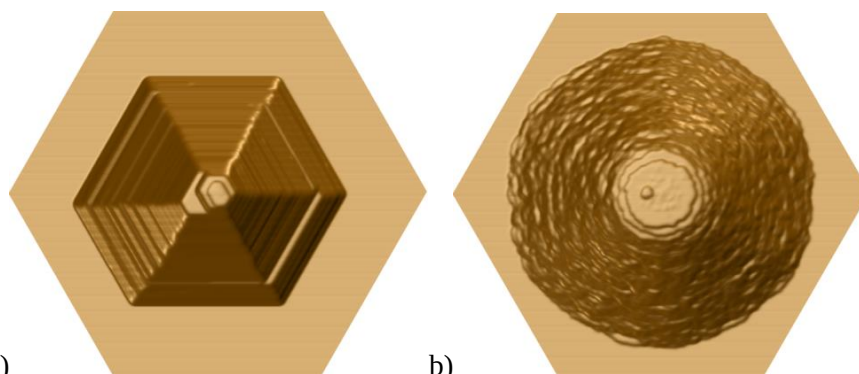
Among the many factors that can initiate the growth of surface structures, defects and their influence on the surface potential energy landscape – and, consequently, on atomic diffusion – are of particular interest. Using the (2+1)D vicinal automaton model [1-4], a powerful simulation tool that enables control over the shape of the surface potential and flexible analysis across different materials, we investigated the role of such defects. By distinguishing surface diffusion from adatom incorporation, we identified key factors governing surface pattern dynamics. A detailed analysis of the diffusion process revealed that defects significantly modify both the character (from local to global) and the shape of the surface energy potential. Furthermore, we found that even slight changes in the probability of atoms attaching to kinks and straight steps can dramatically alter the final morphology of the structures, leading to the formation of cylindrical structures rather than hexagonal nanopillars.

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Acknowledgment

The authors express their gratitude to The Polish National Center for Research and Development (grant no. EIG CONCERT-JAPAN/9/56/AtLv-AlGaIn/2023).



a) b)
Figure 1: Nanopillars obtained by adatom diffusion regulated surface potential of a) local , b) global character.

Modeling Defect-Induced Pattern Formation in Discrete Systems

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We demonstrate how to design subsurface line defects, including screw and edge dislocations, within the (2+1)D Vicinal Cellular Automaton (VicCA) discrete modeling framework [1-4]. The VicCA approach enables the investigation of how deeply embedded structural irregularities dictate macroscopic surface morphology. By decoupling the lattice geometry from the kinetic deposition of adatoms, we show how the internal strain and topological discontinuities of the lattice are 'imprinted' onto the growth process. Our simulations reveal that specific surface formations are not merely stochastic artifacts, but are geometries strictly governed by the long-range influence of subsurface defects. Specifically, we explore how a single, long-range screw defect triggers the continuous winding of terrace layers, creating characteristic hillock patterns. We also demonstrate the emergence of complex surface 'bridges' and saddle points generated by a pair of counter-rotating screw dislocations situated beneath the surface. These results confirm that the VicCA approach effectively captures the topological feedback loop between internal flaws and external pattern formation. By separating these phases, the model avoids the massive computational cost of calculating global elastic relaxation for every newly deposited atom. Instead, the long-range influence of the defect is pre-calculated within the lattice layer, while short-range kinetics are handled in the adatom cloud layer.

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Acknowledgment

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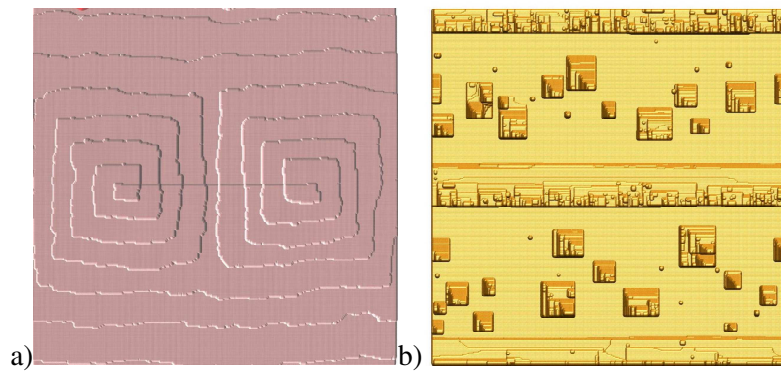


Figure 1: a) Surface morphology induced by a pair of counter-rotating screw dislocations situated beneath the surface. b) Complex pattern of coalesced hillocks emerging atop a defected crystal lattice.

Multiscale Modeling of Stress-Driven Dislocation Formation in SiC Crystal Growth

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Silicon carbide (SiC) is a wide-bandgap semiconductor widely used in high-power and high-temperature electronic devices. However, the growth of large SiC crystals using the physical vapor transport (PVT) method remains challenging due to the formation and propagation of crystallographic defects such as dislocations [1]. These defects are strongly influenced by both atomic-scale growth mechanisms and macroscopic stresses that develop during crystal growth [2].

In this work, a multiscale computational approach is employed to investigate defect formation in SiC during vapor phase deposition and bulk crystal growth. Density functional theory (DFT) is first used to evaluate the thermal stability of the surface steps within a range of high temperatures, and subsequently, molecular dynamics (MD) simulations are used to examine the deposition and nucleation of SiC on off-axis 4H-SiC substrates. The simulations reveal the formation of crystalline SiC through an initial amorphous layer followed by atomic rearrangement into hexagonal stacking structures. Depending on the deposition species, polytype competition between 2H, 4H, and 6H structures are observed, along with the emergence of dislocation within the growing film.

To evaluate macroscopic conditions that promote defect propagation, finite element analysis (FEA) is performed to calculate the normalized resolved shear stress within SiC boules grown by the PVT process. Boule diameters ranging from 2 to 18 inches are considered, with curvature values varying from 0 to 20 mm. For each geometry, the resolved shear stress is evaluated along crystallographic plane orientations between $\theta = 0^\circ$ and 45° . The results show that the critical resolved shear stress of 8 MPa is exceeded for boule diameters greater than 3 inches, with the highest stress concentrations occurring near the boule edge.

These findings suggest that while dislocations may nucleate during the deposition process, stress concentrations arising from boule geometry can drive their propagation during large-scale crystal growth. The combined atomistic and continuum simulations provide insight into how growth conditions and crystal geometry influence defect formation in SiC, offering guidance for optimizing growth processes for large diameter SiC substrates.

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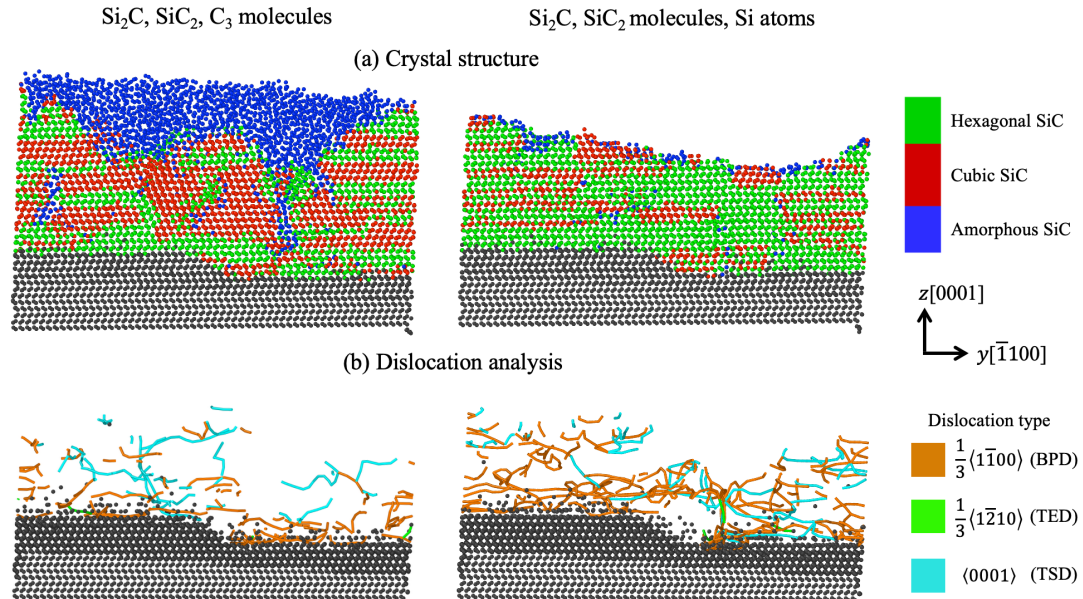


Figure 1: Crystal structure (a) and Dislocation analysis (b) after PVT deposition of Si₂C, SiC₂ and C₃ molecules (left) and Si₂C, SiC₂, molecules and Si atoms (right).

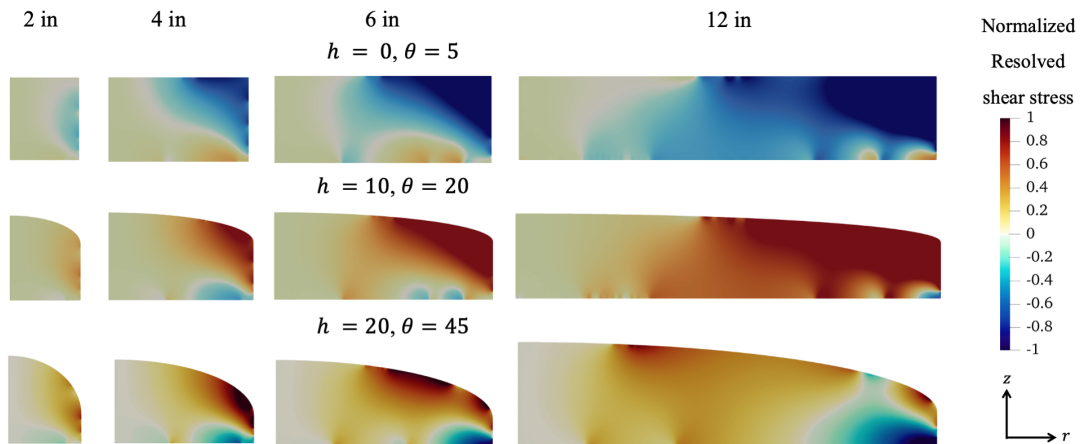


Figure 2: Fields of normalized resolved shear stress (NRSS) for 2 in, 4 in, 6 in, and 12 in boules for different curvature h , and plane orientation θ . The resolved shear stress is normalized by the experimental critical resolved shear stress of 8MPa. NRSS below -1 (compression), or above +1 (tension) denote where CRSS is considered exceeded.

Point Emitter Quantification in Photoluminescence Scans using a Convolutional Neural Network

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Quantum technology device development based on color centers in semiconductors requires simultaneous development of suitable material processing and semiconductor technology processes. One major concern is the impact of such processes on the color center generation yield. The state-of-the-art approach to determine the generation yield employs individual $g^{(2)}$ autocorrelation measurements [1] on many emitters. However, this approach has fundamental drawbacks: The method usually requires color centers arranged in array-shape with advanced tooling like electron beam lithography or a focused ion beam system capable of implanting very small numbers of ions. Especially for lower brightness color center species, the $g^{(2)}$ measurement on enough emitter candidates is extremely time-consuming and it becomes even more challenging in the presence of undesired surface or interface emitters. Therefore, this method is not suitable for in-line characterization accompanying material and technology process development. Alternative known approaches also have drawbacks: Manual counting becomes overwhelming for many emitters and induces human bias. Deconvolution of a given point spread function (PSF) and multi PSF fitting suffer from noisy and distorted images.

In this work, we developed an alternative characterization approach that enables high throughput and fast feedback color center and emitter quantification with good statistics, overcoming the mentioned drawbacks of the state-of-the-art methods: We take advantage from the characteristic brightness of the color center of interest: A self-developed convolutional neural network structure is employed, trained with synthetic training data adapted to the characteristics [2] of the confocal photoluminescence (PL) microscope setup used for this investigation. We demonstrate the extraction of emitter brightness distributions from single PL mappings including surface-related emitters and color centers generated by ion irradiation. We classify the emitters by brightness and validate the method using low temperature PL spectrum measurements, achieving accuracy, precision and recall of about 91 %, 93 % and 89 %, respectively for the detection of silicon vacancy color centers ($V_{Si}(h)$) in 4H-silicon carbide. Finally, we demonstrate that the method is robust against variations in sample surface properties. Compared to the state-of-the-art method, we achieved a characterization speedup by a factor of 50.

While the approach was developed and tested for the quantification of V_{Si} color centers in 4H-SiC, we believe that it could be of interest to other fields of single emitter imaging as well.

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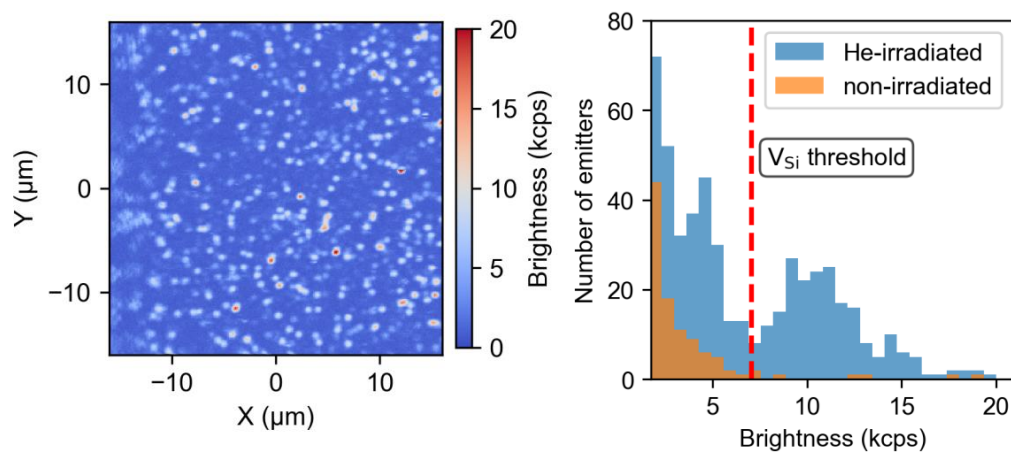


Figure 1: Left: Photoluminescence mapping of a helium ion-irradiated $4H$ -silicon carbide sample. Right: Corresponding emitter brightness distribution (blue) and a reference brightness distribution of a non-irradiated sample. The dashed red line indicates the brightness threshold for V_{Si} color center quantification. Emitters exceeding this brightness can be assumed to be V_{Si} color centers.

10

III-nitrides III

THURSDAY · 3 SEPTEMBER 2026

09:10–10:30

Hall of Mirrors

Chair: František Hájek

PRESENTATIONS

- 10.0** **Takuo Sasaki** INVITED
Unveiling the Dynamics of III-Nitride Surfaces and Interfaces by In Situ Synchrotron XRD
- 010.1** **Tomasz Sochacki**
Growth-mode-induced defects in bulk GaN crystals
- 010.2** **Magdalena Zając**
Dislocation configurations and associated inhomogeneities in bulk GaN

Unveiling the Dynamics of III-Nitride Surfaces and Interfaces by In Situ Synchrotron XRD

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III-nitride semiconductors are expected to play key roles not only in conventional optoelectronic applications but also as fundamental components in emerging quantum technologies, including spintronics, quantum light sources, and topological devices. Despite these technological advances, significant challenges remain in crystal growth. A major issue is the limited understanding of the growth dynamics of surfaces, interfaces, and nanostructures, particularly with respect to atomic structures, strain states, defect behaviors, and compositional variations. In situ synchrotron X-ray diffraction (XRD) provides a powerful approach for accurately characterizing these phenomena, owing to the availability of high-brilliance X-rays that are exceptionally sensitive to lattice variations during growth. We have developed a molecular beam epitaxy chamber for nitride growth at the SPring-8 synchrotron radiation facility and have investigated the growth dynamics of various nitride systems [1,2]. In this presentation, we will highlight representative results on the growth dynamics of III-nitride films and nanostructures.

One of our key research topics is understanding the structure of liquid Ga on epitaxially grown GaN(0001), which is crucial for elucidating nitride growth dynamics and optimizing growth conditions to achieve high-quality GaN films. Although extensive theoretical studies have examined the structure of liquid Ga, it remains unclear whether Ga atoms are randomly distributed or exhibit a specific surface alignment. To probe the atomic arrangement of Ga atoms, we performed in situ XRD during Ga deposition onto the GaN surface at typical growth temperatures. We experimentally confirmed the formation of a Ga bilayer on GaN and quantitatively determined its structural parameters, including interlayer spacing, coverage, and temperature factors [3].

As a recent topic, we have also investigated strain-relaxation behavior during heteroepitaxial InGa_{0.2}N growth on GaN substrates using in situ synchrotron X-ray diffraction reciprocal space mapping. Time-resolved measurements revealed that growth temperature strongly influences both indium incorporation and strain relaxation. Lower growth temperatures promoted higher indium compositions and more rapid strain relaxation, whereas higher temperatures resulted in lower indium incorporation and more pseudomorphic growth constrained by the GaN substrate. These findings provide direct insights into the relationship between growth conditions, alloy composition, and strain evolution, contributing to the optimization of growth processes for high-efficiency nitride optoelectronic devices.

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Acknowledgments

This work was supported by JSPS KAKENHI Grant Number 25K08498.

Growth-mode-induced defects in bulk GaN crystals

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² *Laboratoire Charles Coulomb (L2C), University of Montpellier, CNRS, Montpellier, France*

³ *Fraunhofer Institute for Applied Solid State Physics (IAF), Freiburg, Germany*

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Bulk GaN crystals grown by ammonothermal (Am) and halide vapor phase epitaxy (HVPE) methods evolve through characteristic growth stages: step propagation, hillock formation and hillock coalescence. At the junction of two adjacent hillocks whose macro-steps meet at 120°, a disturbed growth morphology develops — a propeller-type defect or inter-hillock region [1,2]. Here, the structural, electrical and compositional properties of such defects are investigated in undoped Am-GaN and n-type HVPE GaN:Ge crystals using photo-etching, Raman spectroscopy, X-ray topography, Hall effect measurements and ToF-SIMS impurity profiling.

Undoped ammonothermal GaN crystals and undoped/Ge-doped HVPE GaN layers grown on misoriented Am-GaN seeds were studied. Ge doping was introduced via GeCl₄, controlled by the chloride ratio $n_{\text{Ge}}/n_{\text{Ga}}$ [5]. Photo-etching used a modified KSO-D solution under Xe lamp illumination. Raman maps were recorded in backscattering geometry. X-ray topography was performed in transmission (Lang technique, Cu-K α_1). Electrical transport was assessed by van der Pauw/Hall measurements; ToF-SIMS provided impurity depth profiles.

UV optical microscopy revealed enhanced luminescence in inter-hillock regions in all samples (Fig. 1). Raman mapping of the LPP+ mode confirmed systematically reduced free carrier concentration in propeller regions: $\sim 6 \times 10^{17} \rightarrow \sim 3 \times 10^{17} \text{ cm}^{-3}$ (undoped Am-GaN); $\sim 4.3 \times 10^{17} \rightarrow \sim 7.4 \times 10^{16} \text{ cm}^{-3}$ (moderately Ge-doped HVPE GaN); $\sim 1 \times 10^{19} \rightarrow \text{low } 10^{18} \text{ cm}^{-3}$ (highly Ge-doped HVPE GaN) (Fig. 2). Photo-etching produced pronounced depth contrast consistent with these differences. ToF-SIMS confirmed reduced incorporation of dominant unintentional donors in propeller regions — direct evidence for growth-mode-dependent impurity partitioning at hillock junctions. X-ray topography showed no strain contrast in undoped or moderately doped samples, but distinct strain/stress features appeared in highly Ge-doped crystals.

Propeller-type defects are a universal feature of bulk GaN growth by both Am and HVPE methods. They exhibit disturbed morphology, reduced unintentional donor incorporation and lower free carrier concentration than the host crystal. At high Ge doping, they additionally introduce measurable lattice strain. Minimizing the hillock coalescence stage and promoting rapid transition to single-hillock growth are essential for electrically uniform GaN substrates.

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Acknowledgment

This research was supported by the Polish National Science Centre (NCN) through project PRELUDIUM 2021/41/N/ST5/04518, by the National Centre for Research and Development (NCRD) through project LIDER14/0152/2023, and by the Foundation for Polish Science from the funds of the European Funds for Smart Economy (FENG) program, Project International Research Agendas (MAB), Grant No. FENG.02.01-IP.05-M042/25.

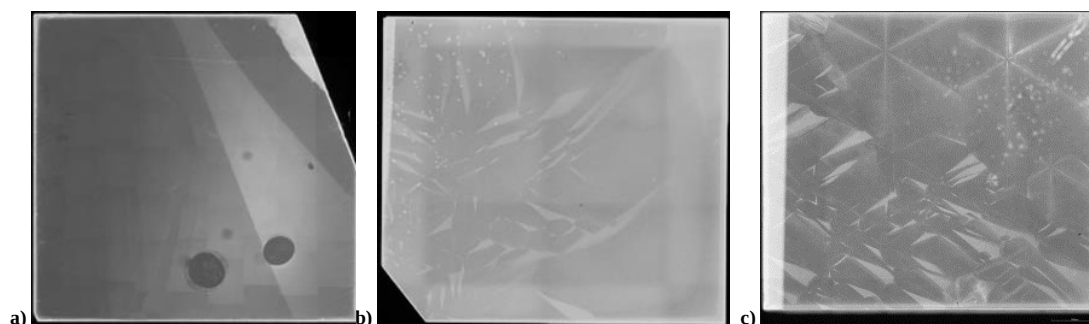


Figure 1. Optical microscopy images under UV illumination of (a) undoped ammonothermal GaN, (b) moderately Ge-doped HVPE GaN and (c) highly Ge-doped HVPE GaN. Enhanced luminescence marks inter-hillock (propeller-type) regions formed at the junction of two merging hillocks with macro-steps oriented at 120° .

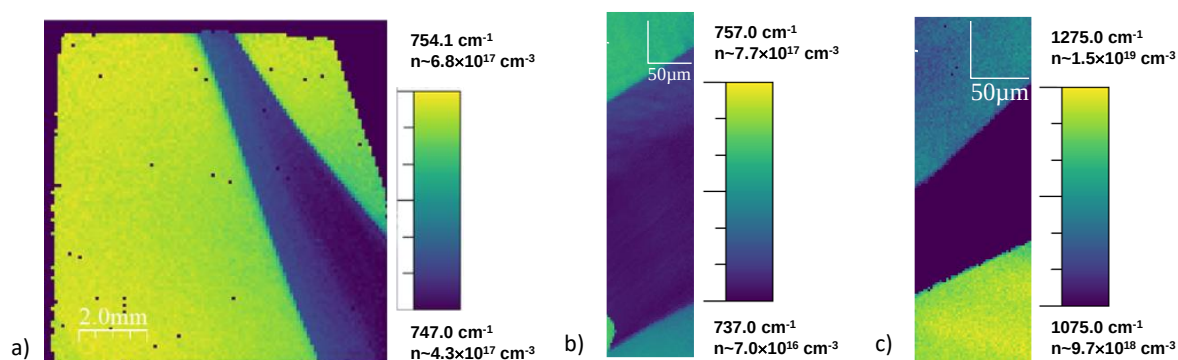


Figure 2. Raman maps of the LPP+ mode for (a) undoped ammonothermal GaN, (b) moderately Ge-doped HVPE GaN and (c) highly Ge-doped HVPE GaN. Free carrier concentrations derived from the LPP+ peak position are given for the host crystal and the inter-hillock (propeller-type) region: (a) $\sim 7 \times 10^{17}$ and $\sim 7 \times 10^{17} \text{ cm}^{-3}$, (b) $\sim 8 \times 10^{17}$ and $\sim 7 \times 10^{16} \text{ cm}^{-3}$, and (c) $\sim 1.5 \times 10^{19}$ and low 10^{19} cm^{-3} , respectively.

Dislocation configurations and associated inhomogeneities in bulk GaN

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Ammonothermal GaN (Am-GaN) substrates, despite very low dislocation density, are not completely free of defects; the presence and spatial distribution of threading dislocations can influence device performance [1]. This work presents a comprehensive study of dislocations and inhomogeneities in Am-GaN using defect-selective etching (DSE), photoetching (PE), X-ray topography, Raman spectroscopy, focused ion beam- transmission electron microscopy (FIB-TEM) and secondary ion mass spectrometry (SIMS).

Two etching methods were applied: DSE using molten KOH–NaOH eutectic with MgO (E+M orthodox etch), and PE based on suprabandgap illumination with K₂S₂O₈ solution. The orthodox etch enables unambiguous discrimination of threading edge ($b = 1/3\langle 1\bar{1}00 \rangle$), mixed ($b = 1/3\langle 1\bar{1}23 \rangle$) and screw dislocations based on pit morphology and depth; FIB-TEM confirmed the pit–Burgers vector correlation. Dislocation density was low (locally 0–10⁴ cm^{−2}) but highly non-uniform, with extended defect-free regions.

Several characteristic dislocation arrangements were identified: isolated pits, hillock-associated clusters, low-angle grain boundaries, herringbone patterns and hexagonal honeycomb defect clusters (HCDs) [2]. DSE revealed HCDs consisting of dislocation bundles at hexagon corners, with a central group of different Burgers vector (Fig. 1). Comparative etching of Ga- and N-polar surfaces demonstrated that HCDs enlarge symmetrically along the [0001] direction, with corner bundles maintaining their hexagonal relationship during growth.

In n-type Am-GaN, PE reveals "dislocation–comet" features associated exclusively with mixed dislocations, with tails oriented toward hillock centers (Fig. 2). Comet formation is attributed to perturbations by atomic-height steps ($\frac{1}{2}c$) at mixed dislocation outcrops, locally disturbing impurity incorporation.

Raman mapping of the LPP[−] mode shows enhanced free-carrier concentration at mixed dislocations (Cottrell atmospheres), while comet regions exhibit slightly reduced concentration. The E₁ mode reveals tensile biaxial strain; SIMS confirms reduced acceptor-type elements (Mg, Mn, Na) at mixed dislocations, with H, O, C and Si remaining uniform.

Correlation of HCDs and dislocation–comet features with growth morphology provides critical insight into their formation mechanisms, constituting a necessary step toward their elimination in Am-GaN substrates.

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Acknowledgment

This research was supported by the Polish National Centre for Research and Development through project LIDER14/0152/2023. This research was also funded by the Foundation for Polish Science from the funds of the European Funds for Smart Economy (FENG) program, Project International Research Agendas (MAB), Grant No. FENG.02.01-IP.05-M042/25.

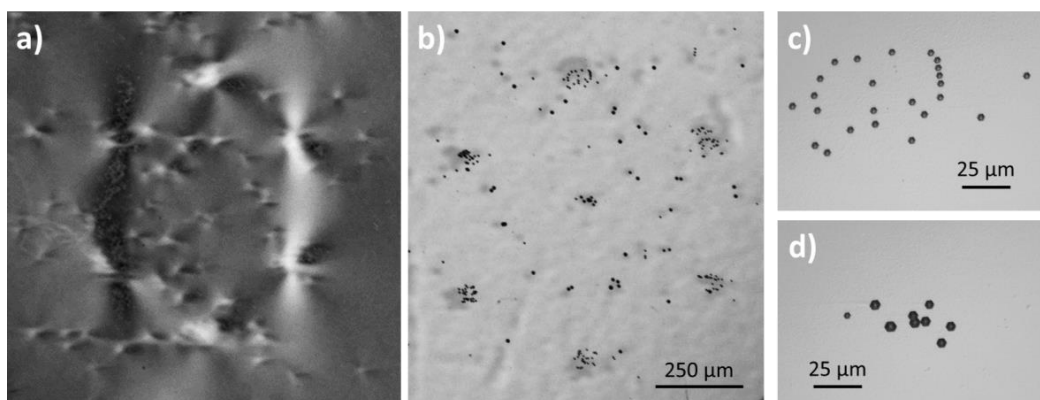


Fig. 1. (a) XRT image and (b-d) DIC optical images of dislocation-related etch pits forming honeycomb-shape pattern.

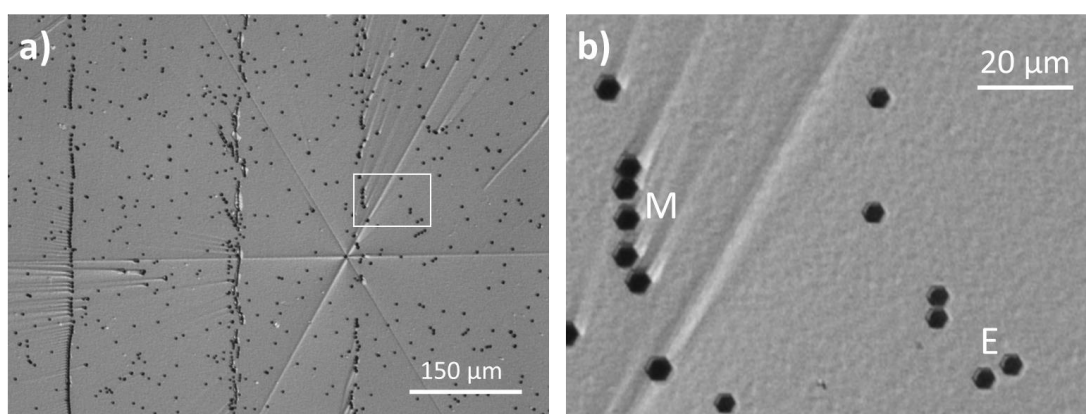


Figure 2: DIC optical images of photoetched and orthodox etched AM-GaN. In (b) an enlarged fragment of image (a) is shown.

11

2D materials

THURSDAY · 3 SEPTEMBER 2026

11:00–12:40

Hall of Mirrors

Chair: Sławomir Kret

PRESENTATIONS

- 11.0** **Daniel Prochowicz** INVITED
Understanding and mitigating defects in lead halide perovskites for robust solar cells
- 011.1** **Izabela Rogala**
Moiré patterns in STEM for polytype identification in epitaxial boron nitride
- 011.2** **Igor Prozheev**
Formation of defects in layered boron nitride
- 011.3** **Łukasz Gelczuk**
Controlled Defect Engineering in van der Waals Semiconductors by Ion Implantation: Electrical Characterization by Junction Spectroscopy Techniques and First-Principles Identification

Understanding and mitigating defects in lead halide perovskites for robust solar cells

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Understanding and mitigating defects in lead halide perovskites is critical for improving the performance and long-term stability of next-generation solar cells based on halide perovskites.[1] These semiconducting materials exhibit remarkable optoelectronic properties, but their sensitivity to defects often leads to non-radiative recombination, reducing device efficiency. Defects can originate from vacancies, interstitials, or impurities introduced during synthesis and processing, influencing both bulk and interfacial properties.

Here I will demonstrate recent studies on passivation strategies, including compositional engineering, additive incorporation, and surface treatments, to minimize defect density and enhance charge carrier lifetimes.[2] By combining defect-tolerant material design with targeted passivation approaches, we have achieved significant improvements in device stability under operational conditions. Continued progress in this area is essential for translating the high efficiencies of perovskite solar cells into commercially viable and durable technologies.

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Acknowledgment

D. P. acknowledges the National Science Centre (Grant OPUS 28, No. 2024/55/B/ST5/01268 for financial support)

Moiré patterns in STEM for polytype identification in epitaxial boron nitride

I. Rogala^{1,*}, J. Iwański¹, A. K. Dąbrowska¹, M. Biliska¹, A. Kaleta², S. Kret², J. Binder¹,
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Layered boron nitride (BN) is a wide-bandgap semiconductor (~6 eV) composed of a graphene-like honeycomb lattice with alternating boron and nitrogen atoms. Variations in stacking sequences of these atomic layers lead to polytypism. Among the most common are hexagonal (h-BN, AA' stacking), rhombohedral (r-BN, ABC stacking), and Bernal BN (b-BN, AB stacking). Polytypism influences the optical response of defects and impurities [1] and enables symmetry-dependent phenomena such as piezoelectricity or ferroelectricity [2]. Additional tunability can be introduced through interlayer twists, which visibly manifest as moiré patterns and give rise to effects such as moiré potentials and the ability to localize excitons [3].

In BN grown by metal-organic vapor phase epitaxy (MOVPE) on sapphire, multiple polytypes and twist angles coexist within a single sample. Such complexity makes it challenging to characterize the structure locally. Notably, while moiré patterns can typically be observed in structures consisting of only a few atomic layers, here they are visible in films composed of dozens of atomic layers, where the twists occur between stacks of well-aligned atomic layers. Interestingly, the presence of moiré patterns can also facilitate precise structural identification, in addition to demonstrating the high crystalline quality of epitaxial BN.

Here, we present an analysis method of moiré patterns in epitaxial BN imaged by scanning transmission electron microscopy (STEM) observed in planar view. To accurately measure moiré period sizes, we introduce a Fourier-transform-based filtration. We demonstrate that by correlating neighboring moiré pattern regions, we can identify both polytypes and twist angles within the analyzed area. This method provides a complementary approach to polytype assessment alongside defect-related optical responses [1]. Such precise characterization of the underlying atomic structure deepens our understanding of the growth process, paving the way for obtaining polytype-pure samples, growing structures with tailored twist angles, and enabling reliable interpretation of defect-related properties.

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Acknowledgment

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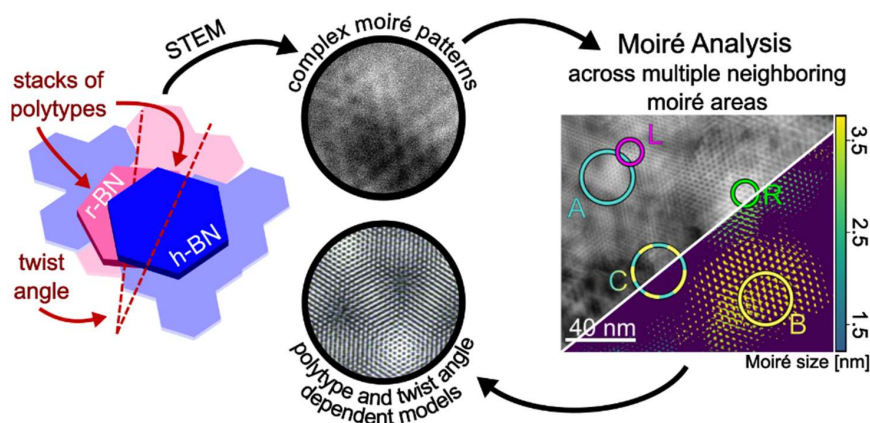


Figure 1: A schematic overview of the moiré pattern analysis. The first panel (left) is a model of the sample, highlighting the coexistence of polytypes and angle twists in MOVPE-grown BN. In the second panel (top center) a STEM image of a moiré pattern is shown, its complexity indicates presence of at least three twisted stacks of layers. A clear Moiré pattern was obtained using the HAADF detector, with a convergence semi-angle of 9.5 mrad and a collection semi-angle range of 16–97.5 mrad, enabling the detection of Bragg disks on detector ring. These conditions maximize the contrast of the Moiré pattern while maintaining relatively high spatial resolution. Next panel (right) depicts the moiré analysis by combining a portion of the STEM image with a moiré period map for the region around area (C) from the previous panel. Analysis of the twist-angle variation from region (L) to (R) indicates that area (A) is composed of r-BN stacks twisted by 4.27° . Further comparison of regions (A–C) reveals that region (C) contains three r-BN stacks, with two of them rotated by 4.27° and 2.17° relative to the third. The corresponding atomic model is provided in the final panel (bottom center).

Formation of defects in layered boron nitride

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Layered boron nitride (BN) is a promising material for development of single-photon emitters or mutable spin defects. However, one of the fundamental challenges is the control of defects formation and mass production of high-quality layered BN material. Development of Metal Organic Vapor Phase Epitaxy with varying growth conditions allows to grow large surface-area BN layers with specific structural defects [1]. Ion beams can be used for controlled production of defects in these layers [2]. And positron annihilation spectroscopy allows to study and characterize vacancy-type defects. [3]

In this work we study BN samples with layers grown in varying conditions. As-grown, neutron-irradiated and N-implanted samples were measured with a slow positron beam. Figure 1 shows preliminary positron results. The data fall in three buckets, those representing as-grown epitaxial BN, V_B^- -related defects and bigger “vacancy clusters”. The lack of pristine BN reference complicates the analysis of defect concentrations. However, N-implantations and neutron irradiations create V_B^- defects, with N-implanted samples appearing to reach saturation positron trapping ($[V_B^-] > 5 \times 10^{18} \text{ cm}^{-3}$). The positron data clearly indicates the presence of big open-volume defects with a possible distribution of $V_B\text{-nH}$ or $V_B\text{-V}_N$ complexes in agreement with previously reported results. [1] Future *ab initio* calculations may provide more insights into the nature of these defects.

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Acknowledgment

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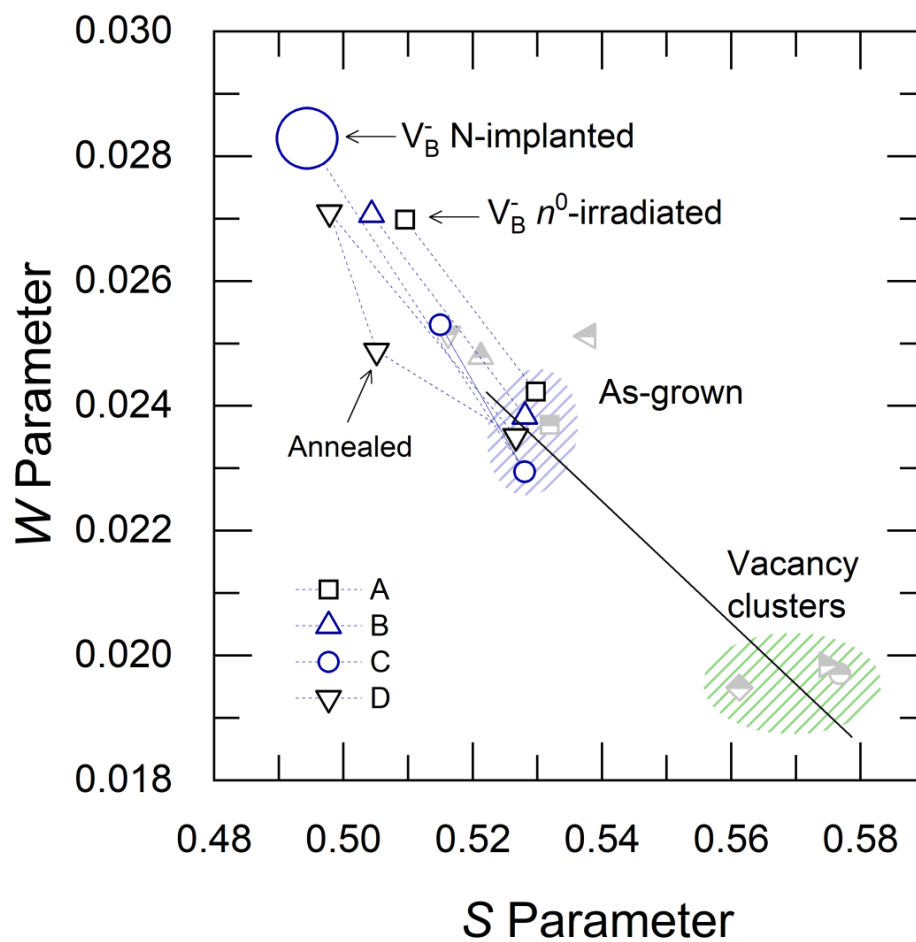


Figure 1: Relative S and W parameters measured in BN samples. The dashed lines illustrate the trends in the V_B^- formation data. Green shaded area illustrates averaged annihilation parameters linked to vacancy clusters. The solid line is used to guide the eye in the positron data moving to bottom-right corner of the plot.

Controlled Defect Engineering in van der Waals Semiconductors by Ion Implantation: Electrical Characterization by Junction Spectroscopy Techniques and First-Principles Identification

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Layered van der Waals (vdW) semiconductors, particularly transition metal dichalcogenides (TMDs), have attracted intense interest for next-generation electronic and optoelectronic devices. Their performance is critically influenced by intrinsic and extrinsic point defects, which act as carrier traps, recombination centers, and scattering sites [1]. This work focuses on the identification and controlled engineering of electrically active deep-level defects in both pristine and ion-implanted bulk TMD crystals, combining junction spectroscopy techniques (JSTs), such as deep level transient spectroscopy (DLTS) with first-principles calculations based on density functional theory (DFT).

The experimental study (see examples in Fig. 1) includes bulk crystals of popular MX₂ family (M = Mo or W; X = S, Se, or Te), as well as other selected layered vdW compounds (e.g. InSe, SnSe, ReSe₂, ...). For sufficiently thick, quasi-bulk samples, vertical Schottky barrier diodes were fabricated, enabling the formation of a well-defined depletion region analogous to that in classical bulk semiconductors. Under these conditions, capacitance-based transient spectroscopy allows determination of activation energies, capture cross sections, and defect concentrations in the 80–400 K temperature range. In pristine crystals, dominant deep electron traps are consistently observed and correlated with native point defects such as vacancies, antisites or interstitials [2]. The strong agreement between experimental and computational results validates the computational approach and enables identification of the microscopic origin of the experimentally observed defect levels, as summarized in Table 1. The validated DFT methodology was then applied to calculate the charge transition levels of defects in monolayer MX₂ systems, which are experimentally challenging to probe using DLTS [3].

In addition to native defects, controlled point defects were introduced by low-energy ion implantation. Helium ions (primarily 60 keV, with doses in the range of 1–4×10¹² cm⁻²) generate vacancy-related defects and defect complexes without inducing amorphization. Systematic variation of implantation energy and dose enables investigation of dose-dependent defect formation and transition from isolated vacancies to other defect configurations. The experimentally extracted deep-level parameters are compared with calculated charge transition levels, enabling reliable microscopic assignment of native and implantation-induced centers.

The proposed approach significantly expands the defect database for bulk vdW semiconductors and establishes ion implantation as a reproducible and tunable tool for defect engineering. The combined experimental–theoretical framework provides a pathway toward controlled tailoring of deep-level spectra in layered materials, relevant for contact optimization, charge transport control, and the development of defect-based quantum functionalities [4].

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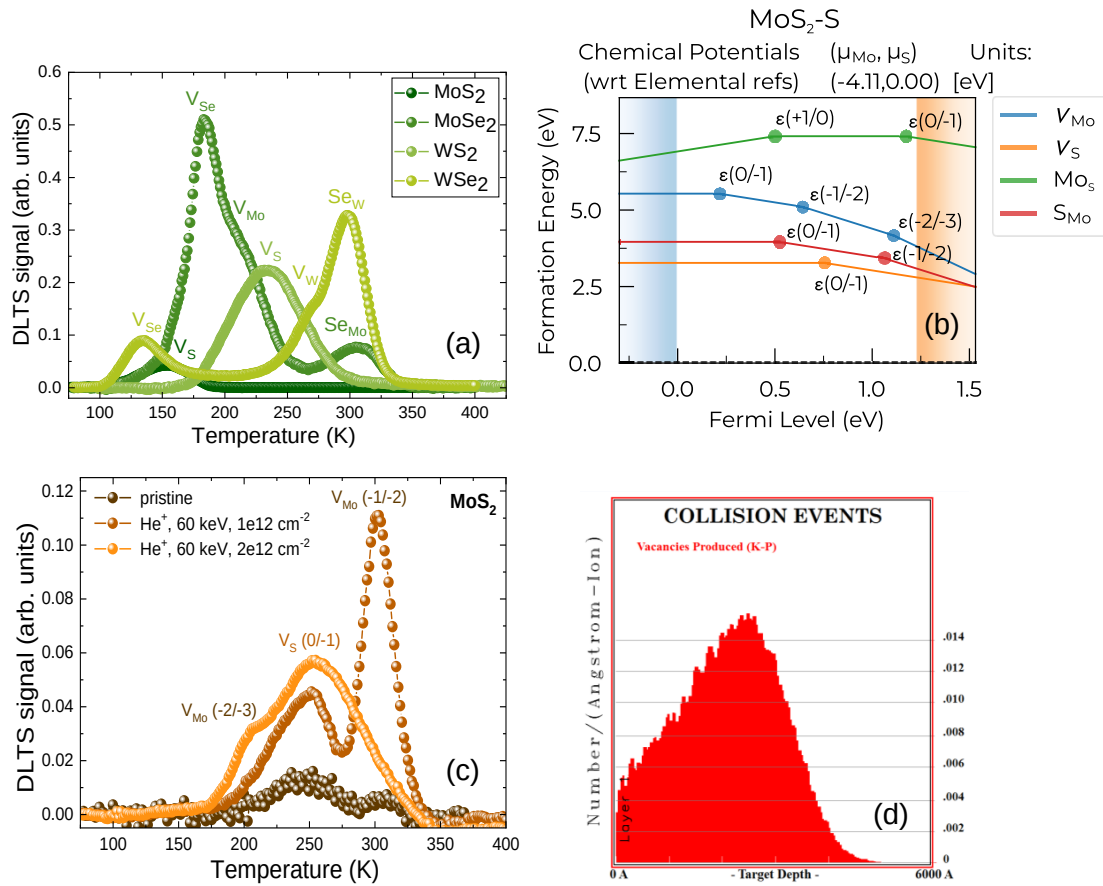


Figure 1: (a) Standard DLTS spectra of bulk MoS₂, MoSe₂, WS₂ and WSe₂ crystals, (b) DFT calculated formation energies of point defects in MoS₂, (c) exemplary DLTS spectra of MoS₂ before and after ion implantation, (d) the ion implantation damage results. (vacancy generation).

Table 1: Comparison of the charge transition levels of defects obtained by DLTS and DFT.

Sample	Transition level [DLTS] (eV)	Transition level [DFT] (eV)	Defect origin
MoS₂	0.35	0.36	V _S (0/-1)
MoSe₂	0.15	0.13	V _{Se} (0/-1)
	0.40	0.44	V _{Mo} (-1/-2)
	0.57	0.59	Se _{Mo} (0/-1)
WS₂	0.33	0.34	V _S (0/-1)
WSe₂	0.14	0.12	V _{Se} (0/-1)
	0.52	0.49	V _W (-1/-2)
	0.59	0.65	Se _W (0/-1)

POSTERS

Poster Session

TUESDAY · 1 SEPTEMBER 2026

17:00–19:00

Erasm Majewski Hall

PRESENTATIONS

P1	Ivana Capan Silicon vacancy in 4H-SiC studied by Laplace - DLTS	P10	Maciej Wojcik Strain and Moiré pattern analysis in wurtzite GaAs – rock-salt (Pb,Sn)Te core-shell
P2	Grzegorz Nowak Effects of oxygen plasma treatment on p-type GaN investigated with Scanning	P11	Min Huang Interface Engineering of Cleaved Facets via Nitrogen Plasma for High-Reliability GaN
P3	Imad Belabbas (a+c) edge dislocation with m-line in wurtzite GaN: core configurations,	P12	Weining Qian Investigation on the Formation Mechanism and Suppression of Linear defects in 4H-SiC
P4	Dorota Janaszko Misfit dislocation network in CdTe/ZnTe radial nanowires – TEM and MD/MS study	P13	Rajan Bharti Multimodal identification of electrically active defects in GaInP
P5	Qingna Wang Impact of sidewall defects on efficiency of miniaturized short-wavelength AlGaIn deep	P14	Rezwana Sultana Optimization Strategy of Hf ₂ ZrO ₂ Thin Film Formation at Room Temperature by
P6	Xiaofang Ye Quantitative evaluation of the correlation between crystal defects and optical	P15	Guiying Shen Investigation of oval defects in InAs homoepitaxy layer grown by MOCVD
P7	Sławomir Kret Structural and cathodoluminescence study of ZnAl ₂ O ₄ on sapphire formed during the	P16	Thamires Soares Intrinsic Defects and Defect-Related Optical Emission in Natural
P8	Marcin Kryśko The calculation of strain tensor of epitaxial layers of any kind of symmetry deposited	P17	Yu Wang Improvement of radiation resistance of GaAs solar cell with InGaAs/GaAsP
P9	Lorenzo Rigutti Compositional Metrology of Atom Probe Applied to Semiconductors		

Silicon vacancy in 4H-SiC studied by Laplace - DLTS

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Point-like defects in wide-bandgap semiconductors have attracted significant attention for quantum-technology applications, particularly as qubits and single-photon emitters. Among these defects, the silicon vacancy (V_{Si}) in SiC is one of the most studied. The negatively charged states of V_{Si} have been comprehensively investigated using low-temperature photoluminescence (PL), electron paramagnetic resonance (EPR), and optically detected magnetic resonance (ODMR). In 4H-SiC, the silicon vacancy gives rise to well-known PL lines commonly referred to as V1 (*h*-site) and V2 (*k*-site) [1]. In addition, V1 has a high-temperature companion labeled V1'.

High-energy particle irradiation and ion implantation introduce electrically active defects into SiC, including the V_{Si} , which creates two deep levels in the bandgap. These levels, known as S1 and S2, have been assigned to different charge-state transitions of V_{Si} at the *h* and *k* sites, corresponding to the ($-3/=-$) and ($=/0$) transitions, respectively [2].

In this work, 1 and 2 MeV proton irradiation was used to introduce V_{Si} defects into 4H-SiC samples. Laplace-DLTS measurements were employed to analyze the S1 (0.40 eV) and S2 (0.70 eV) levels. Furthermore, we investigate the correlation between the PL lines V1/V1' and the Laplace-DLTS signals S1/S2. These findings contribute to a deeper understanding of the S1 and S2 defects and their potential relevance for quantum-technology applications.

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Effects of oxygen plasma treatment on p-type GaN investigated with Scanning Kelvin Microscopy

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Oxygen plasma treatment of p-GaN surface damages performance of subsequently deposited ohmic contacts. Areas subjected to plasma do not conduct current. Normally such degradation is not desirable. In some cases plasma damage can be used to create insulating regions replacing dielectric insulation in electronic devices.

The exact mechanism of ohmic contact degradation caused by oxygen plasma is not clear¹. Bombardment with energetic ions can lead to sputtering damage, oxygen removal/deposition and oxide formation. Generation of donor-like point defects like nitrogen vacancies, O on nitrogen sites and various complexes can lead to insulating or even inverted surface.

We have performed Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM)² surface potential measurements on p-type GaN affected by oxygen plasma.

GaN p-type morphology, measured with AFM, does not change after oxygen plasma treatment, but surface potential measured with KPFM differs between plasma-treated and not-plasma-treated regions. The difference depends on plasma duration and intensity.

During KPFM measurements we found that potential difference between treated and not-treated regions does not depend on electrical potential applied to n-type layer. This confirms that the p-type layer after plasma treatment is electrically continuous.

We have also measured change of surface potential (Surface Photovoltage, SPV) after illumination with UV light³. In both oxygen plasma-treated region and non-treated region SPV signal is negative, indicating downward band bending at the surface. This proves that oxygen-treated p-type surface does not contain n-type layer.

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(a+c) edge dislocation with m-line in wurtzite GaN: core configurations, dissociation and climb

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III-nitride semiconductors have become technologically relevant materials in nowadays modern society due to their broad range of electronic and optoelectronic applications [1]. One interesting thing with these materials is their possession of a continuous alloy system with tunable direct energy bandgaps, spanning a large part of the electromagnetic spectrum from ultraviolet to infrared through visible [1]. This key feature allowed for a successful application of III-nitride materials in producing light emitting devices, such as light-emitting diodes (LEDs), laser diodes (LDs) and UV detectors [1].

The growth of III-nitride semiconductors is usually achieved by heteroepitaxial techniques, on structurally and thermally mismatched foreign substrates [2]. This leads to the formation of a high concentration of structural defect, namely dislocations [3]. The latter were proven to have a harmful impact on the performances of III-nitrides based electronic devices. In the last two decades dislocations, of different types and running along different directions, were extensively investigated in III-nitride materials [4]. Among these dislocations, those along the m-direction, i.e. $\langle 10\bar{1}0 \rangle$, were the least studied, although they were recently proven to play a role in the interfacial strain relaxation in InGaN systems [5].

In the present work, core configurations and electronic structure of the (a+c) edge perfect dislocation, with a line parallel to the m-direction, were predicted by using computer atomistic simulations in wurtzite GaN. The latter are based on density functional theory (DFT). The obtained structural models were used to propose mechanisms for the dissociation and the climb of the (a+c) edge perfect dislocation at the atomic scale. Structural features related to dissociation and climb, predicted by atomistic simulations, were confirmed by high resolution scanning transmission electron microscopy observations at the GaN/InGaN interface [6,7].

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Acknowledgment

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Misfit dislocation network in CdTe/ZnTe radial nanowires – TEM and MD/MS study

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Here, we present the results of our investigations into highly mismatched core/shell nanowires (NWs), in which the lattice mismatch exceeds 6.2%, grown by molecular beam epitaxy (MBE). Two groups of NWs were distinguished. Among them are partially relaxed NWs with core diameters of 60–90 nm and an asymmetric shell with a thickness of 10–50 nm. The misfit dislocation network at the core/shell interface was investigated using HR-STEM images and is clearly visible in the GPA amplitude image (Fig. 1a). Perpendicular and oblique cross-sections of the investigated samples were prepared to determine the nature of the dislocation cores. The distances between dislocations were measured in both oblique cross-section images taken along the [110] zone axis and in plane-view images along the [112] zone axis. It was found that the dislocation spacing at the CdTe/ZnTe interface in the analyzed nanostructures depends on the shell thickness, symmetry, and core diameter.

Molecular dynamics (MD) and molecular statics (MS) simulations of the investigated structures were performed. We used the LAMMPS [1] package equipped with two types of interatomic potentials to ensure the highest accuracy. System parameters were optimized to determine the dislocations' characteristics as well as their core atomic configuration, stability, and probability of formation. The simulation results are in good agreement with the experimental microscopy observations. The need for these simulations arises from the practical challenges encountered during microscopic investigations. Regions affected by dislocations are not clearly visible at high resolution because of the uneven distribution of atoms in the atomic columns and their displacements. The dislocation extraction algorithm (DXA) [2] applied to the relaxed CdTe/ZnTe core/shell supercell allows 3D visualization of the dislocation lines present at the core/shell interface. This visualization enables a more direct interpretation of the TEM data, which are always obtained as 2D projection of the complex 3D core/shell nanowire geometry.

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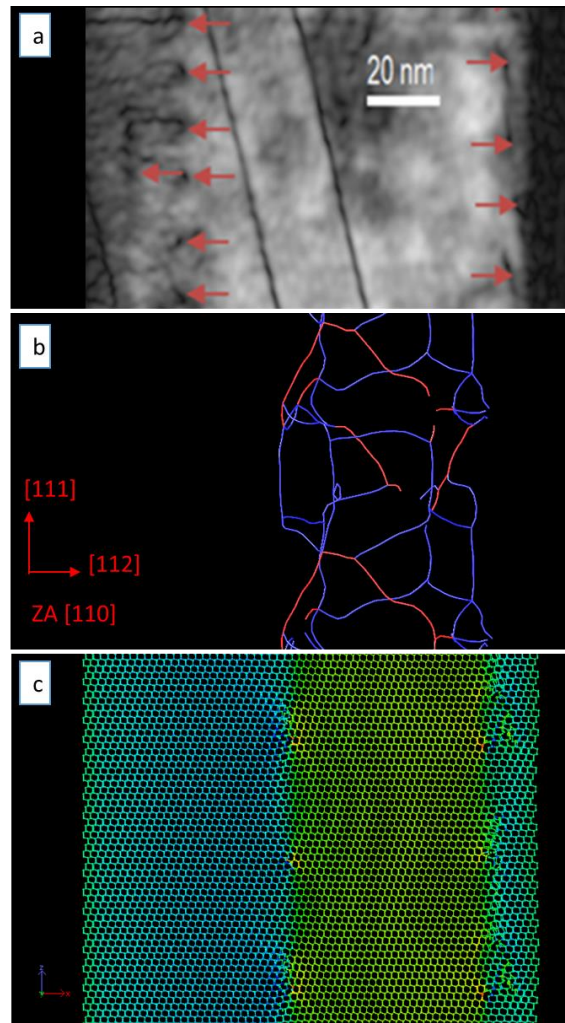


Figure 1: (a) experimental image of amplitude of 112 beam, where arrows point misfit dislocation cores. (b) simulated 3D misfit dislocation network visualization after Dislocation analysis (DXA), and (c) xx strain of the core/shell CdTe/ZnTe nanowires.

Impact of sidewall defects on efficiency of miniaturized short-wavelength AlGaIn deep ultraviolet light-emitting diodes

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Extremely low internal quantum efficiency (IQE) and light extraction efficiency (LEE) remain the primary bottlenecks for short-wavelength AlGaIn deep ultraviolet (DUV) LEDs.[1] The former arises from the extremely high dislocation densities in high-Al-content epitaxial layers, which leads to strong nonradiative recombination, while the latter stems from the predominance of TM-polarized emission in high-Al-content AlGaIn and strong absorption on the p-type side, both of which hinder light extraction. Although device miniaturization and the introduction of reflective inclined sidewalls can effectively tailor photon propagation and enhance LEE,[2] the accompanying sidewall damage and surface defects impose increasingly severe adverse effects. The resulting enhancement of Shockley-Read-Hall (SRH) recombination may partially or even completely offset the optical gains from LEE improvement.[3]

In this study, we examined the impact of sidewall defects on the performance of miniaturized, short-wavelength (~250 nm) deep ultraviolet (DUV) LED arrays using a combination of theoretical simulations and experimental validation. By integrating a surface recombination velocity (SRV) model into our simulations, we compared the emission performance both with and without the effects of sidewall recombination. Our findings (Figure 1a) indicate a noticeable decline in optical output when sidewall recombination is considered: the output power drops from 39.2 mW to 36.4 mW at 350 mA, representing a 7.7% reduction and highlighting the substantial influence of sidewall defects on carrier recombination. Notably, the current-voltage (I-V) characteristics remain largely unaffected, suggesting that the observed optical degradation arises primarily from carrier diffusion to sidewall defects, where nonradiative recombination occurs, rather than from a decrease in injection efficiency. Additionally, far-field radiation patterns (Figure 1b) demonstrate a reduction in overall emission intensity across various angles. Experimental measurements are consistent with these results, confirming that miniaturized devices suffer significant IQE degradation due to pronounced nonradiative recombination caused by sidewall defects.

These findings demonstrate that under device miniaturization, sidewall defects induced nonradiative recombination plays an increasingly prominent role in limiting device efficiency, in addition to the geometrically induced LEE enhancement. Although sidewall passivation has been extensively studied in conventional blue and green miniaturized LEDs, in applications where improving LEE is the primary objective, the miniaturization scale and array design must still be carefully balanced to avoid performance losses caused by sidewall defects.

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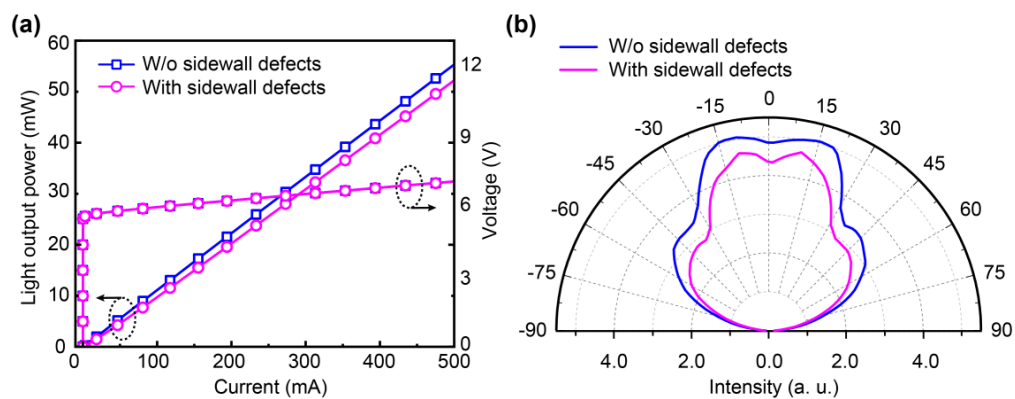


Figure 1: (a) Simulated light output and I-V characteristics of the 250-nm UVC LEDs with and without the sidewall defect model. (b) Corresponding far-field angular emission patterns at a driving current of 350 mA.

Quantitative evaluation of the correlation between crystal defects and optical properties in semi-insulating 4H-SiC wafers

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Semi-insulating 4H silicon carbide (4H-SiC) is a pivotal material for high-precision optical components, especially in the rapidly expanding virtual reality (VR) and augmented reality (AR) near-eye display market, owing to its ultra-wide bandgap, broad optical transparency, and exceptional thermal conductivity [1]. However, crystal defects introduced during bulk crystal growth, including micropipes, carbon inclusions, threading dislocations, and surface scratches [2], can lead to significant optical failures such as light leakage, wavefront aberration, and transmission loss. These issues directly degrade VR/AR imaging quality and user experience [3]. Despite the importance of these effects, a systematic and quantitative correlation between crystal defects and critical optical performance metrics of 4H-SiC for optical device applications has yet to be established.

In this work, a series of optical non-destructive characterization methods, including bright-field (BF) optical microscopy and photoluminescence (PL) imaging, were employed to precisely locate typical optical defects in 4H-SiC wafers. Subsequently, multi-type defects were quantitatively analyzed using fixed- and variable-angle microscopic angle-resolved spectroscopy (μ -ARS), confocal Raman spectroscopy, and high-precision Fizeau interferometry, complemented by finite-difference time-domain (FDTD) and COMSOL multiphysics simulations to elucidate the physical mechanisms underlying defect-induced optical degradation. Three key quantitative findings were obtained: (1) A typical optical phase difference of approximately $\lambda/20$ was measured between micropipe-containing regions and adjacent defect-free areas, revealing the intrinsic origin of light leakage and wavefront aberration in optical lenses; (2) Carbon inclusions were unambiguously identified via characteristic disordered carbon Raman peaks, and induce a broadband transmission loss of up to 12% in the 400 to 1600 nm spectral range; (3) Threading dislocations and scratches cause significant 2° - 5° shift and about 2 fold broadening of angular-resolved scattering peaks, and a linear model between dislocation density and 1064 nm optical propagation loss is established with a goodness of fit R^2 of 0.987.

Our work establishes a quantitative mapping between multiple types of crystal defects and optical performance degradation in 4H-SiC through a combination of experimental characterization and numerical simulation. It elucidates the underlying physical mechanisms of defect-induced optical failures and provides critical guidance for achieving high optical quality in SiC crystal growth, as well as for non-destructive quality control of VR/AR optical components.

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Structural and cathodoluminescence study of ZnAl_2O_4 on sapphire formed during the growth of ZnO nanowires in a carbothermal process

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Zinc oxide nanowires (ZnO NWs) stand out with a high piezoelectric coefficient, biocompatibility, chemical stability, non-toxicity, and low-cost synthesis, making them promising for nanoscale energy harvesting and sensing applications.

An Al_2O_3 – ZnAl_2O_4 –ZnO heterostructure was synthesized using a modified carbothermal process on a-plane and m-plane sapphire substrates [1,2]. In the initial stage, a ZnAl_2O_4 spinel buffer layer forms via interdiffusion of Zn atoms, what results with creation a new crystalline phase develops within the subsurface region of the sapphire while maintaining a coherent crystallographic relationship, both in orientation and lattice matching, with the host matrix. The spinel interlayer, with a thickness ranging from 2 to 10 nm, subsequently serves as a structural template for the nucleation and oriented growth of ZnO NWs. The NWs grow perpendicular to the surface on a-plane substrate, whereas they are inclined at approximately 60° on m-plane sapphire (Fig. 1a,b). However the grow direction is always [0001] (fig 1c). To explain crystallographic origin of this phenomena high resolution transmission electron microscopy studies revealed that the spontaneously formed spinel layer preserves a well-defined epitaxial relationship with sapphire. The epitaxial relationship between sapphire, spinel and ZnO is as follow: $[0001]_{\text{sapphire}} \parallel [1-21]_{\text{spinel}} \parallel [-12-10]_{\text{ZnO}}$. Additionally in the case of sapphire and spinel, the crystallographic directions are $[-1-2101]_{\text{sapphire}} \parallel [-113]_{\text{spinel}}$.

According to GPA analysis, the in-plane strain (ϵ_{xx}) is approximately 2% between sapphire and spinel, whereas the out-of-plane strain (ϵ_{yy}) at the spinel–ZnO interface is even lower, below 1%. Furthermore, the (111) planes of spinel are parallel to the (0001) planes of ZnO, which correspond to the preferential [0001] growth direction of the ZnO nanowires Fig 2 and facilitate nearly defect-free nanowire growth (Figure 1c,d).

Cathodoluminescence studies reelevated the optical activity of the ZnAl_2O_4 layer, revealing a dominant near-band-edge emission at 3.75 eV and a pronounced negative thermal quenching effect, with emission intensity increasing steadily from 7 K to room temperature (Figure 3). The temperature dependence of the integrated emission intensity follows a thermal activation model with an activation energy of 15.3 ± 0.7 meV. The spontaneous formation of an optically active spinel buffer during carbothermal growth thus provides a new route for designing functional oxide heterostructures for future optoelectronic applications.

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Acknowledgment

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Figure 1 Vertically oriented ZnO nanowire on an $a\text{-Al}_2\text{O}_3$ $[11\bar{2}0]$ substrate and at an angle of 60° to an $m\text{-Al}_2\text{O}_3$ $[10\bar{1}0]$ substrate; (c) HRTEM image of the ZnO NW tip with a diameter of approximately 10 nm; (d) magnified view of the frame from (c).

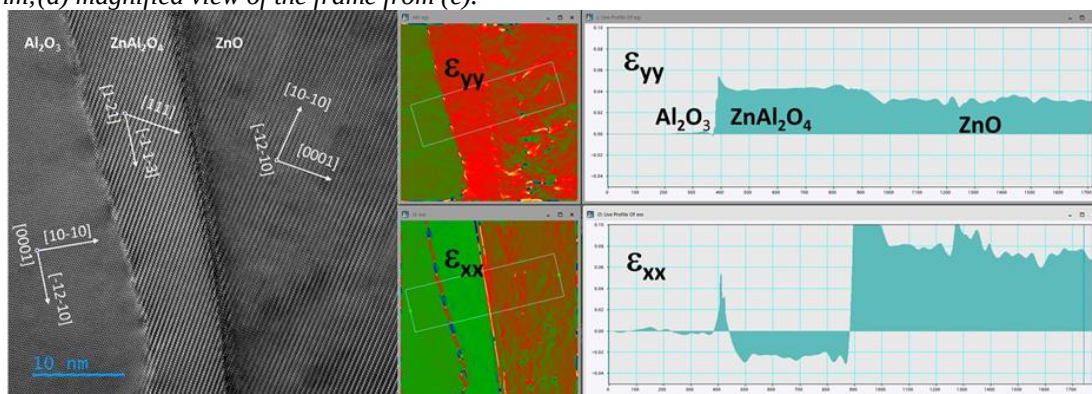


Figure 2: Atomic structure of the sapphire/spinel/ZnO interface formed during endotaxy in the carbothermal process on an m -plane Al_2O_3 substrate. HRTEM image with indicated crystallographic directions. Maps and line profiles of the lattice distortion tensor components ε_{xx} and ε_{yy} .

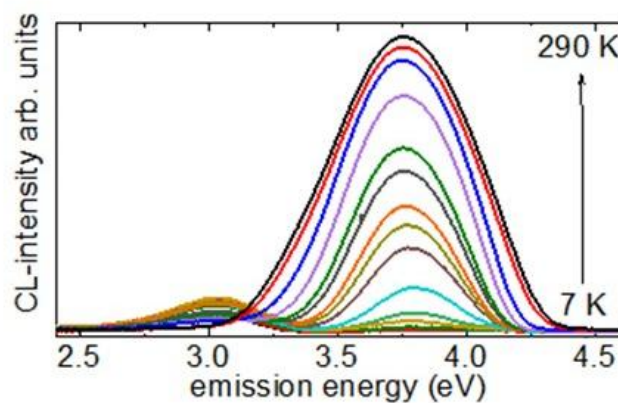


Figure 3: temperature dependence of CL spectra showing negative thermal quenching effect

The calculation of strain tensor of epitaxial layers of any kind of symmetry deposited on any orientation of a substrate

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The relaxed (unstrained) lattice parameters of crystalline alloys depend on the proportions of the individual components in the alloy. This property makes it possible to determine these proportions (chemical composition) if the lattice parameters are measured using high-resolution X-ray diffraction (HRXRD).

In practice, we often deal with epitaxial layers made of such alloys deposited on a substrate with different lattice parameters. In such a situation, the layer becomes strained. The lattice parameters of the layer change. The change in the parameters parallel to the surface, resulting from lattice mismatch, also forces a change in the remaining parameters in accordance with the elastic properties of the layer material.

The deformation of the layer lattice is usually described using the strain tensor ε_{ij} , containing 9 components, including 6 independent ones. This strain must be taken into account when calculating the chemical composition based on measurements of lattice parameters. In that case, knowledge of all components of the strain tensor is required.

In the case of a crystal with high symmetry and where the surface normal is parallel to one of the axes of the unit cell, strain occurs only in directions parallel and perpendicular to the surface (Fig. 1a). Then only the diagonal components ε_{xx} , ε_{yy} , and ε_{zz} of the strain tensor are non-zero, and the calculations are relatively simple. However, in the general case also the shear components ε_{xy} , ε_{yz} , and ε_{xz} of the strain tensor become non-zero (Fig. 1b), which makes the calculations more complicated.

For the case of crystals with cubic symmetry, this problem was solved in work [1], whereas for crystals with hexagonal symmetry in work [2].

In this work, we show a method for calculating the components of the strain tensor for epitaxial layers made of crystals of any symmetry and for any surface orientation.

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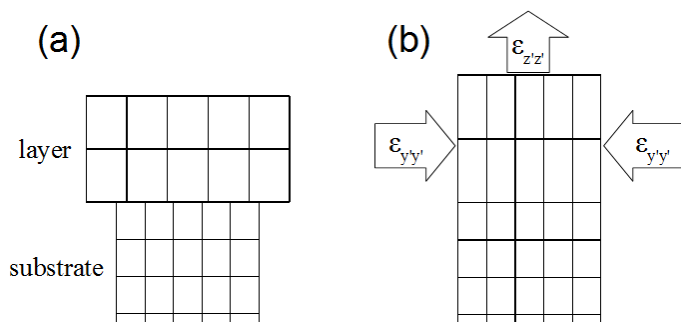


Figure 1: Straining of a layer made of high crystal symmetry where the surface normal is parallel to the unit cell axis. Only diagonal components of the strain tensor are non zero. Rectangular unit cells remain rectangular. (a) before straining (b) after straining

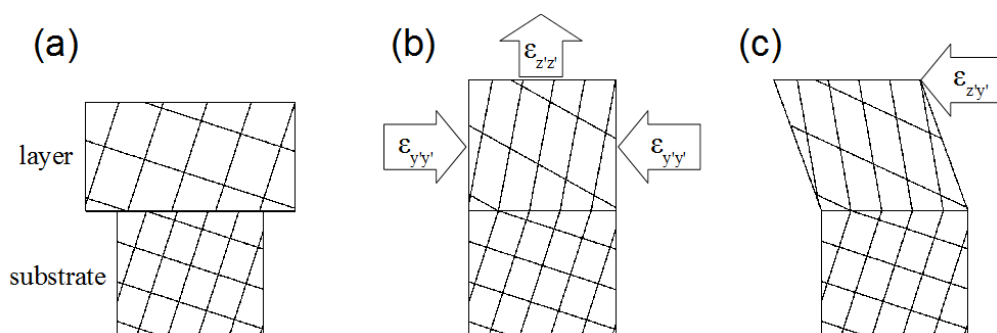


Figure 2: Straining of a layer deposited on the substrate of any surface orientation, artificially divided into two steps. (a) Situation before straining, (b) strain in the directions parallel and perpendicular to the surface only, (c) shear components of the strain tensor become non zero - tilt of the lattice.

Compositional Metrology of Atom Probe Applied to Semiconductors

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Laser-assisted Atom Probe Tomography (La-APT) is nowadays a common technique for the assessment of 3D-resolved chemical composition in semiconductors. This capability is extremely useful for the study of defects, as it can target impurity density and distribution in, and can even succeed in imaging extended defects in specific cases. Two decades after its introduction, APT has demonstrated a unique potential for the study of defect-related issues in semiconductor materials and devices, and in a growing list of inorganic non-metallic solids.

A crucial and often underestimated issue with APT is its accuracy in compositional measurements of non-metallic systems. In this work we remind some of the aspects potentially leading to compositional biases and underlining in particular the role of the surface electric field in governing the different physical-chemical phenomena that enable the measurement. We list and review possible mechanisms of specific losses, as well as the methods for assessing a compositional bias and proposing possible correction methods. Finally, it gives examples of compositional biases in APT of semiconductors and some take-home messages for semiconductor scientists and microscopy users [1].

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Strain and Moiré pattern analysis in wurtzite GaAs – rock-salt (Pb,Sn)Te core-shell nanowires grown by molecular beam epitaxy

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Topological crystalline insulators (TCIs) belong to extensively investigated research area of topological quantum matter. The interest in TCIs stems from the presence of topologically protected Dirac states on high symmetry surfaces of TCI crystals. (Pb,Sn)Te solid solution is one representative of TCIs, with topological phase occurring above some critical Sn content (30 – 35 %, depending on temperature). Since topologically protected states in TCIs are surface properties, we have studied this material in quasi one-dimensional nanowire (NW) geometry providing high surface-to-volume ratio. To further enhance the surface-related properties we have chosen to investigate core-shell NW heterostructures with wurtzite (WZ) GaAs cores and (Pb,Sn)Te shells [1] instead of uniform NWs [2,3]. Core-shell NW heterostructures have been grown by molecular beam epitaxy using two distinct MBE systems dedicated to III-V, and IV-VI semiconductors. The interface structure of WZ-GaAs/(Pb,Sn)Te NWs is investigated using wide range of characterization techniques, such as high resolution transmission electron microscopy (HR-TEM), scanning transmission electron microscopy (STEM) and geometric phase analysis (GPA). We have shown that (Pb,Sn)Te can be successfully grown as continuous full or half-shells on the sidewalls of GaAs NWs, which provides opportunity for investigation of topological surfaces of TCIs in the tubular geometry. Moiré fringes analysis provides alternative method of strain analysis to the geometric phase analysis method. Dislocation distance varies between different regions of the shell, suggesting that shell structure is less strained near the edge and more strained away from the discontinuous shell fragment. Analysis of the acquired TEM and STEM images reveals that the shell consists of several connected fragments rather than a single continuous structure, which contribute to unevenly distributed strain across the shell. Moiré fringes distances in perpendicular direction are significantly shorter than in the parallel direction. This is a direct result of much higher mismatch in the lattice parameters of the shell and the core materials in parallel and perpendicular directions.

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Interface Engineering of Cleaved Facets via Nitrogen Plasma for High-Reliability GaN Laser Diodes

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The mirror facets of GaN-based edge-emitting lasers are typically fabricated by cleaving, inherently possessing a high density of dangling bonds. These unsaturated bonds readily react with ambient species, forming complex precipitates that increase optical absorption and degrade the crystal lattice during laser operation, thereby significantly lowering the threshold for catastrophic optical mirror damage (COMD). This study investigated the effects of plasma treatments on the interface quality between the cleaved facet and mirror coating, and their impact on the device performance of GaN-based edge-emitting lasers.

X-ray photoelectron spectroscopy analysis revealed that Ar plasma treatment induced negligible chemical modification, whereas O plasma treatment led to severe gallium oxidation, as indicated by a 0.5 eV positive shift in the Ga 2p binding energy. In contrast, N plasma treatment effectively repaired nitrogen vacancies and facilitated the formation of new Ga–N bonds, evidenced by a pronounced 0.4 eV positive shift in the Ga 2p peak and a minor 0.1 eV positive shift in the N 1s peak. These results confirmed successful surface passivation and stoichiometric restoration. Furthermore, transmission electron microscopy combined with Fast Fourier Transform analysis corroborated these findings, showing that N plasma treatment yielded a highly ordered crystalline interface, while Ar and O plasma treatments produced amorphous or distorted surface layers. The superior interface quality achieved via N plasma treatment directly enhanced device performance. Compared to untreated devices and those subjected to Ar or O plasma treatments, lasers with N-plasma-treated facets demonstrated a lower threshold current and higher slope efficiency. Moreover, N-plasma-treated devices displayed significantly improved resistance to COMD under high current injection, distinguishing them from Ar- and O-plasma-treated samples.

These results confirm that N plasma treatment is an effective technique for preparing high-quality, robust mirror facets, essential for the development of high-performance GaN-based laser diodes.

Investigation on the Formation Mechanism and Suppression of Linear defects in 4H-SiC Epitaxial Growth

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Abstract:

Silicon carbide (SiC) epitaxial layers are fundamental to the development of next-generation high-power and high-frequency electronic devices. However, the presence of crystallographic defects, particularly Shockley-type stacking faults (SFs) which often appear as linear features, critically compromises device performance and reliability [1]. This work systematically investigates the formation mechanism and evolutionary behavior of linear defects in 4H-SiC homoepitaxial layers. To precisely trace the origin and propagation of these defects, a multi-step analytical approach was employed involving the sequential removal of the epitaxial layer. By examining the as-grown surface, the partially etched layer, and the interface after complete epilayer removal, the root sources of the defects were definitively identified at the substrate/epilayer interface and within the bulk substrate. Furthermore, the influence of key process parameters on linear defect formation was comprehensively evaluated. Through systematic optimization of the epitaxial growth rate, in-situ etching conditions, and growth temperature, a direct correlation was established between these parameters and the nucleation and extension of the linear defects. The findings reveal that a controlled balance of growth kinetics and meticulous surface preparation are essential for effective defect suppression. Ultimately, by implementing the optimized process conditions informed by this defect evolution study, the density of linear defects was significantly reduced, leading to a substantial improvement in the crystalline quality of the SiC epitaxial films.

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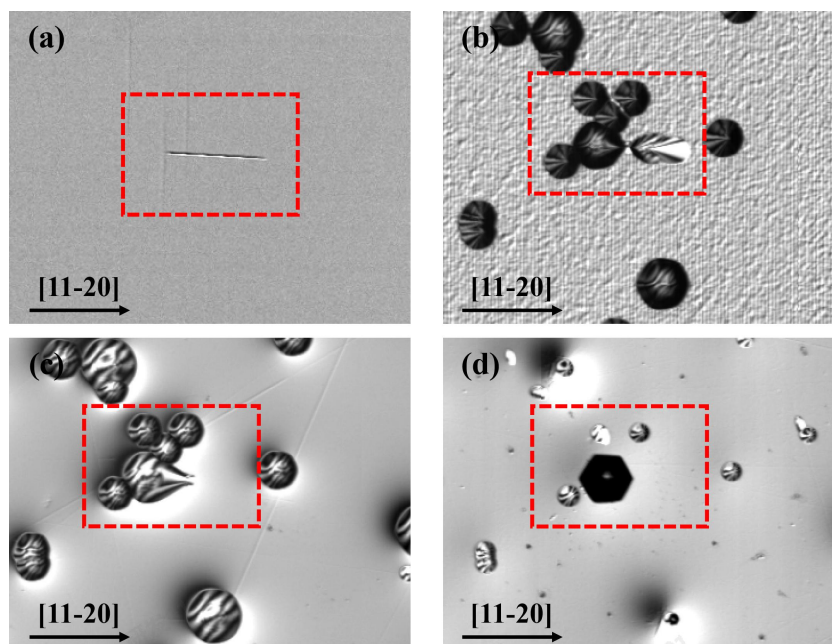


Figure 1. Tracing the origin of linear defects in the epitaxial layer (epilayer thickness $\sim 12 \mu\text{m}$, SICA)
 (a) Surface morphology of the defects on the as-grown Si-face epilayer; (b) Morphology of the defects at the same location after KOH etching; (c) the defects morphology at the same location after removing approximately $5 \mu\text{m}$ of the epilayer by CMP, followed by KOH etching; (d) the defect morphology on the substrate surface at the same location after complete removal of the epilayer ($\sim 12 \mu\text{m}$) by CMP, followed by KOH etching

Multimodal identification of electrically active defects in GaInP

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Gallium indium phosphide (GaInP) is a promising material for high-efficiency red LEDs owing to its direct bandgap of 1.85 eV and lattice matching with GaAs. However, when device dimensions are reduced below 100 μm , the external quantum efficiency decreases markedly [1,2]. This size effect is widely attributed to non-radiative recombination at defect-rich mesa sidewalls, yet the electrical characteristics of the responsible defects remains poorly understood. Here, we combine DLTS, admittance spectroscopy, TCAD simulations and DFT calculations to identify and correlate bulk and interface defects in GaInP.

A 1 μm -thick GaInP epilayer was grown on GaAs by MOVPE and used to fabricate both Schottky and metal–oxide–semiconductor (MOS) test structures (Fig. 1). DLTS measurements were performed using a filling pulse of 0 V, an emission pulse of -2 V and a pulse width of 10 ms. The DLTS spectra reveal several deep bulk levels, $E_c - 0.47$, $E_c - 0.76$ and $E_c - 0.96$ eV in n-GaInP, and $E_v + 0.48$ and $E_v + 0.77$ eV in p-GaInP (Fig. 2). The $E_c - 0.96$ eV level lies close to mid-gap and has previously been identified as an efficient recombination centre [3], making it a likely contributor to the efficiency loss observed in scaled devices. Most of the remaining deep levels are consistent with phosphorus-vacancy-related defects and may also contribute to carrier compensation [4-6]. Although DLTS provides valuable information on bulk defects, its sensitivity to near-interface defects is limited.

To investigate defects near the semiconductor surface, planar MOS capacitors incorporating thermally deposited Al_2O_3 layers of 15–33 nm were fabricated to emulate mesa sidewalls. The capacitance–voltage characteristics exhibit non-ideal behaviour. The 1 MHz Capacitance reaches only 20–25% of the oxide capacitance at +4 V. Strong frequency dispersion is also observed (Fig. 3), while oxide-thickness-dependent analysis reveals a persistent depletion width of approximately 75 nm (Fig. 4). These observations indicate strong surface-potential pinning by a high density of near-interface defects.

TCAD Ginestra® simulations reproduce the experimental characteristics using two defect families [7]. The first consists of shallow pinning states located 0.1–0.2 eV below the conduction band, concentrated at the interface with densities approaching $5 \times 10^{21} \text{ cm}^{-3}$ and decaying within the first 5 nm of GaInP. The second consists of oxide border traps confined to the first nanometre of Al_2O_3 , with densities of approximately $5 \times 10^{19} \text{ cm}^{-3}$, accounting for the observed frequency dispersion. A similar defect landscape is found in p-type GaInP, with equivalent states referenced to the valence band (Fig. 5). DFT calculations associate the shallow pinning states with phosphorus vacancies related defects which is consistent with observations from literature [8], suggesting a possible origin for the high-density interface defects (Fig. 6). Together, these results establish a comprehensive defect spectrum for GaInP, identifying deep recombination centres, shallow pinning states and oxide border traps as key targets for passivation. The findings provide important insights into the mechanisms governing sidewall recombination and restoring efficiency in sub-100 μm optoelectronic devices.

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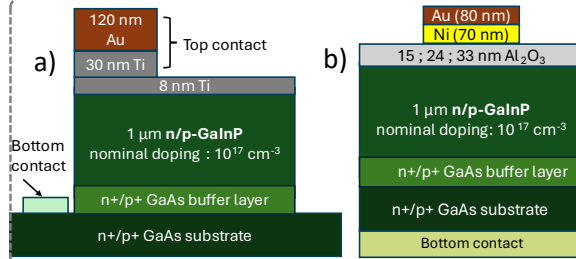


Fig.1 Cross-sectional schematic of the n-doped (Si)/p-doped (Mg) (a) Schottky & (b) MOS structure. The bottom contact is Au/Ge/Au/Ni/Au and Ti/Pt/Au for n and p-doped structures, respectively.

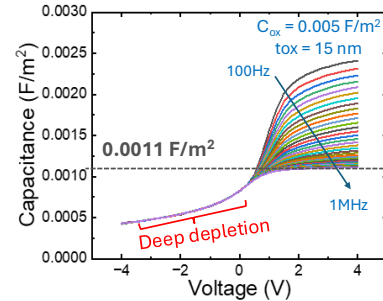


Fig.3 Multi-frequency CV response for the n-doped GaInP MOS structure at room temperature (22°C) measured in a dry air and dark environment.

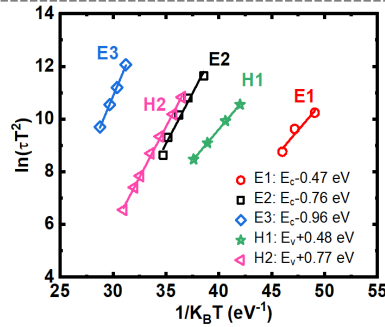


Fig.2 Arrhenius analysis of DLTS data for n and p-doped GaInP Schottky diodes. Three defect levels E1, E2 and E3 with trap densities $3.27 \times 10^{13} \text{ cm}^{-3}$, $6.94 \times 10^{13} \text{ cm}^{-3}$ and $1.10 \times 10^{15} \text{ cm}^{-3}$ respectively, were identified for n-doped GaInP while two defect levels H1 and H2 with trap densities $2.07 \times 10^{13} \text{ cm}^{-3}$ and $8.65 \times 10^{13} \text{ cm}^{-3}$, were identified for p-doped GaInP.

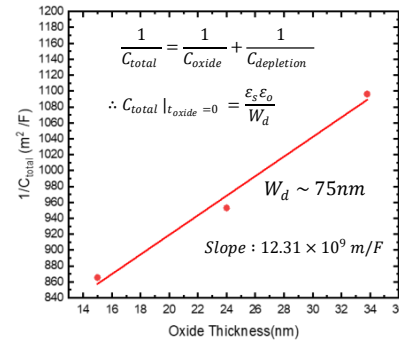


Fig.4 Reciprocal capacitance at +4 V (1 MHz) versus Al_2O_3 thickness, used to estimate surface potential pinning induced depletion width.

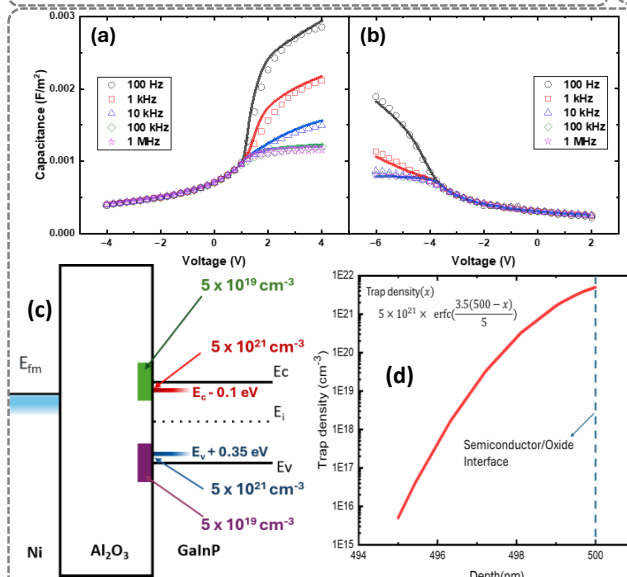


Fig. 5 Multi-frequency C–V characteristics at 50 °C for (a) n-GaInP/ Al_2O_3 and (b) p-GaInP/ Al_2O_3 MOS capacitors, showing agreement between experimental results and TCAD simulations. (c) Extracted trap distributions across the upper and lower halves of the bandgap. (d) Spatial distribution of high-density GaInP pinning states near the interface used for simulations for n & p GaInP.

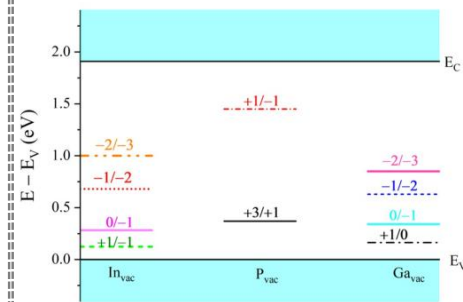


Fig.6 DFT calculations indicate intrinsic Phosphorus-vacancy-related defects introduce two charge-transition levels within the bandgap, located near the conduction- and valence-band edges. Among the intrinsic vacancies considered, phosphorus vacancies exhibit the lowest formation energies, indicating a higher likelihood of occurrence. The shallow level near the conduction/valence band is consistent with the high-density shallow defect states identified by admittance spectroscopy, suggesting phosphorus vacancies related defects as a plausible atomic origin of the interface pinning defects.

Optimization Strategy of $\text{Hf}_{1-x}\text{Zr}_x\text{O}_2$ Thin Film Formation at Room Temperature by Pulsed-DC Sputtering Using a Periodic Layer-by-Layer Deposition Process and Electrical Evaluation in Ru-Based MOS Devices

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The recent finding of ferroelectricity in doped HfO_2 thin films deposited through atomic layer deposition (ALD) has revitalized research in the semiconductor industry due to their remarkable CMOS compatibility and potential applications in advanced memory and logic devices [1]. Among the various dopants, Zr plays a crucial role in stabilizing the ferroelectric phase of HfO_2 and become a material of great interest for further development of memory devices [2, 3]. In this work, $\text{Hf}_{1-x}\text{Zr}_x\text{O}_2$ thin films were deposited using a novel pulsed-DC magnetron sputtering technique, designed to emulate an ALD-like process through a layer-by-layer periodic deposition sequence. The resulting samples HZ-4L and HZ-8L represent films containing four and eight ZrO_x layers, respectively, while HZ-8L(T) represents a similar HZ-8L structure with slightly thicker ZrO_x layer. Fig. 1(a) and (b) present the cross-sectional TEM image of the HZ-4L and HZ-8L(T), respectively. The corresponding EDS line profiles are displayed in Fig. 1(c) and (d). Fig. 1(a) and (c) confirmed homogeneous diffusion of ZrO_x within the HfO_x matrix, forming a ~ 36 nm $\text{Hf}_{1-x}\text{Zr}_x\text{O}_2$ layer with ~ 3.6 nm interfacial SiO_x layer at room temperature. In contrast, Fig. 1(b) and (d) reveal a layer-by-layer stacking and periodic distribution of alternative $\text{HfO}_x/\text{ZrO}_x$ layers, indicating incomplete interdiffusion. The SiO_x thickness increases to ~ 4.9 nm. Complete interdiffusion is possible when the thickness of each ZrO_x layer is less than 2.5 nm. But for HZ-8L(T), as the thickness of each ZrO_x layer is ~ 3.8 nm, complete mixing does not take place. Fig. 2(a)-(c) display GI-XRD analysis of the films. Fig. 3(a)-(c) show the Ru/ $\text{Hf}_{1-x}\text{Zr}_x\text{O}_2$ /Si device structure, C-V and G-V characteristics, respectively. HZ-8L exhibits the highest accumulation capacitance, whereas HZ-8L(T) shows reduced accumulation capacitance due to the thicker interfacial layer. The extracted interface state density (D_{it}) and C-V hysteresis are shown in Fig. 4(a). The thicker interface layer in HZ-8L(T) lowers D_{it} , resulting in reduced hysteresis. The forward and backward current-voltage (I-V) sweeps (Fig. 4(b)) indicate that leakage current increases with higher ZrO_x content. Fig. 4(c) shows a reduction in the leakage current minima (I_{min}) for HZ-8L(T), which can be attributed to the low D_{it} of HZ-8L(T). Periodic layer-by-layer sputtering enables controlled incorporation of ultrathin ZrO_x within HfO_x , forming a tunable $\text{Hf}_{1-x}\text{Zr}_x\text{O}_2$ stack at room temperature. The films exhibit reduced leakage current and minimized C-V hysteresis, indicating improved dielectric quality. Although Ru electrodes have been studied on HfO_2 , their electrical behavior on such novelly sputtered $\text{Hf}_{1-x}\text{Zr}_x\text{O}_2$ films remains unexplored to date. These results demonstrate the viability of sputtered $\text{Hf}_{1-x}\text{Zr}_x\text{O}_2$ ferroelectric films and the compatibility of Ru electrodes for next-generation non-volatile memory applications.

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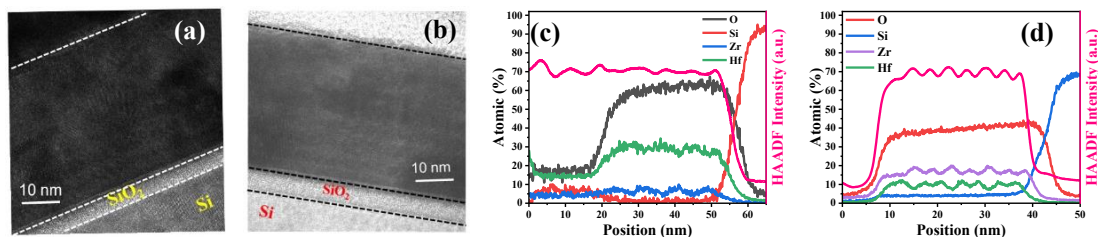


Fig. 1. Cross-sectional TEM images of (a) HZ-4L and (b) HZ-8L(T). The corresponding EDS line profile of (c) HZ-4L and (d) HZ-8L(T).

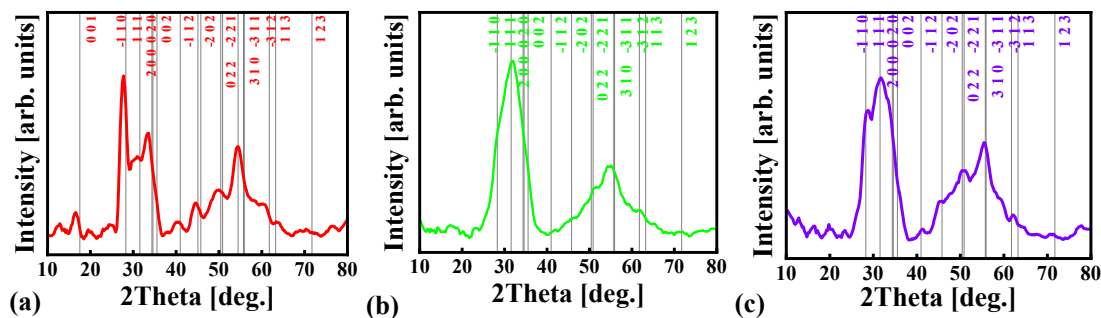


Fig. 2. GI-XRD scan of (a) HZ-4L (b) HZ-8L and (c) HZ-8L(T). XRD pattern showing reflections consistent with monoclinic HfO_2 , with peak positions indexed according to the reference file (00-034-0104). Although the diffraction peak correspond to the characteristic Miller indices of monoclinic HfO_2 , the peaks are markedly broadened and partially overlapping. The presence of broad halos at positions associated with crystalline phases reflecting poor crystallographic ordering and a pronounced amorphous character.

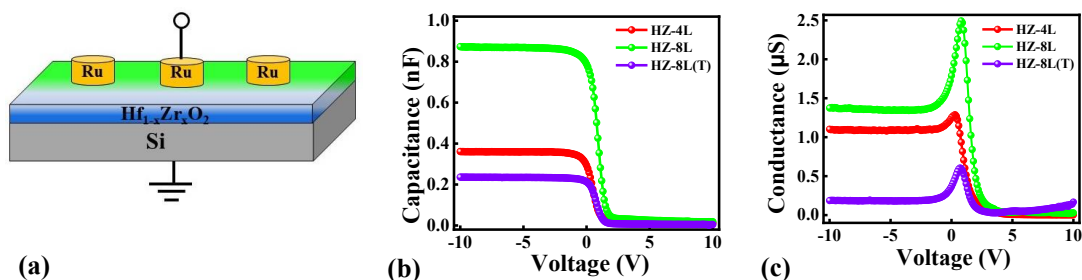


Fig. 3. (a) Scheme of $\text{Ru}/\text{Hf}_{1-x}\text{Zr}_x\text{O}_2/\text{Si}$ MOS structure. (b) C - V sweep from inversion to accumulation region and (c) corresponding conductance plots.

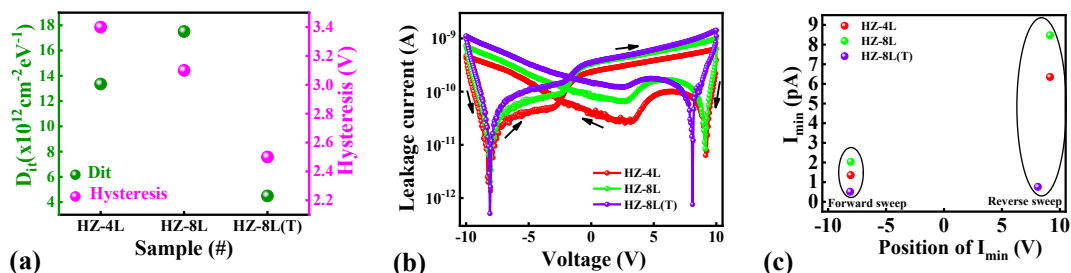


Fig. 4. (a) Comparison of interface state density and C - V hysteresis of HZ-4L, HZ-8L and HZ-8L(T). (b) Comparison of gate leakage current behavior with change in sweep direction. Sweep direction is illustrated by arrows indicating forward (-10 V to $+10$ V) and reverse ($+10$ V to -10 V) sweep. (c) Value of $I_{\min}$ during forward and reverse sweep for all the samples.

Investigation of oval defects in InAs homoepitaxy layer grown by MOCVD

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Indium arsenide (InAs) features a direct bandgap of 0.36 eV and a lattice constant that closely matches GaSb, rendering it a preferred material for type-II superlattice infrared detectors. A critical challenge for achieving high-performance devices lies in mitigating the various defects, including dislocations, stacking faults, polycrystalline regions, and oval defects, that persistently form within the requisite high-quality epitaxial layers. Among these, oval defects represent a common type of defect in epitaxial growth. However, current research has largely focused on gallium-containing materials such as GaAs [1-2] and InGaAs [3], while relatively few studies have addressed the nature of such defects in InAs epilayers [4]. The internal structure and formation mechanism remain poorly understood, necessitating further study to develop effective mitigation strategies for achieving high-quality, oval defect-free InAs epilayers.

In this study, a 2-inch, un-doped InAs substrate oriented in the [100] direction was used for the growth of a 1- μ m-thick InAs epilayer via metal–organic chemical vapor deposition (MOCVD). The morphology and internal structure of oval defects were characterized using optical microscopy (OM), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Energy-dispersive X-ray spectroscopy (EDS). As shown in Figure 1, optical microscopy reveals that the typical oval defect exhibits an elliptical protrusion containing a hexagonal pit. The hexagonal feature is oriented with one of its symmetry axes parallel to the [110] direction. In Figure 2(a), SEM imaging reveals a hexagonal feature comprising a slightly raised, platform-like surface with a core particle at its center. The dark-field image in Figure 2(b) shows the (110) cross-sectional morphology, delineating the epi-layer/substrate and core particle/epi-layer interfaces. Figure 2(c) demonstrates consistent crystal orientation between substrate and epitaxial layer, indicating good lattice matching. The electron diffraction pattern in Figure 2(d) exhibits a polycrystalline ring pattern, attributed to atomic misalignment at the core particle/epi-layer interface. To investigate the defect origin, EDS point analyses are conducted at the seven positions marked in Figure 2(b). The results in Table 1 reveal significant As depletion within the substrate region directly beneath the defect, particularly at position 7. Based on these results, it is proposed that the oval defect formation is initiated by a localized compositional deviation in the substrate, which introduces stress during epitaxial growth and ultimately leads to the oval defect generation.

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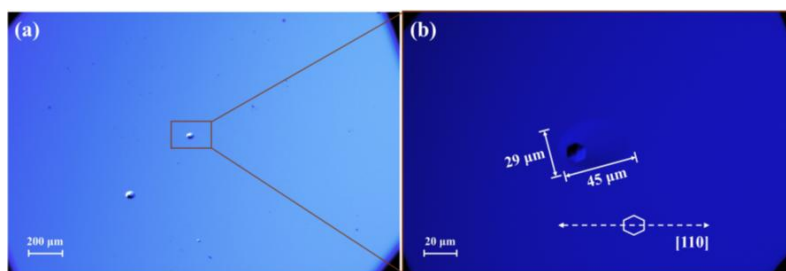


Figure 1. Surface morphology of oval defects observed by optical microscopy at (a) 50 $\times$ and (b) 500 $\times$ magnification.

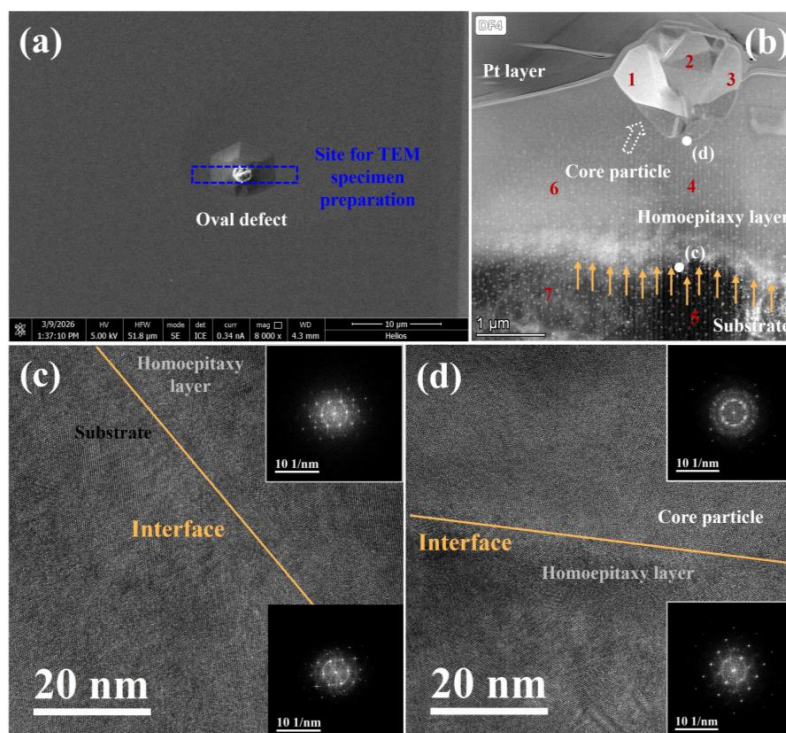


Figure 2. (a) SEM image of an oval defect surface morphology; (b) cross-sectional dark-field TEM image of the oval defect along the (110) plane; (c) and (d) HRTEM images and corresponding electron diffraction patterns acquired from the two interfaces marked in (b).

Table 1. EDS point analysis results

Element	Position						
Atomic fraction	1	2	3	4	5	6	7
In (%)	51.97	52.19	51.81	52.07	58.96	52.05	57.72
As (%)	48.03	47.81	48.19	47.93	41.04	47.95	42.28

Intrinsic Defects and Defect-Related Optical Emission in Natural Two-Dimensional Talc

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Two-dimensional materials have emerged as promising platforms for defect-based optoelectronic and quantum photonic applications, where optically active defects can act as localized light emitters [1]. While defect-related emission has been widely explored in synthetic van der Waals materials, naturally occurring layered minerals remain largely unexplored despite their structural diversity and wide band gaps [2].

Among these materials, phyllosilicates such as talc ($\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$) represent an appealing class of natural layered systems that can be exfoliated down to few layers and may host intrinsic defects and trace-element impurities formed during geological growth [3]. These defects can strongly influence the local electronic structure and may give rise to optically active states.

Here we investigate intrinsic defects and their associated optical response natural talc crystal (Fig. 1a) exfoliated onto SiO_2/Si substrates. The morphology and thickness of the flakes are characterized by optical microscopy (Fig. 1b) and atomic force microscopy (Fig. 1d). Photoluminescence spectroscopy reveals defect-related emission features, while nano-X-ray fluorescence (nano-XRF) mapping provides spatially resolved elemental information (Fig. 1e), enabling the identification of trace elements such as Fe and their correlation with optically active regions (Fig. 1f).

Our results provide new insights into the relationship between intrinsic defects, trace-element incorporation, and optical activity in layered minerals. These findings highlight natural phyllosilicates as an emerging class of materials for studying defect-related optical phenomena in low-dimensional systems.

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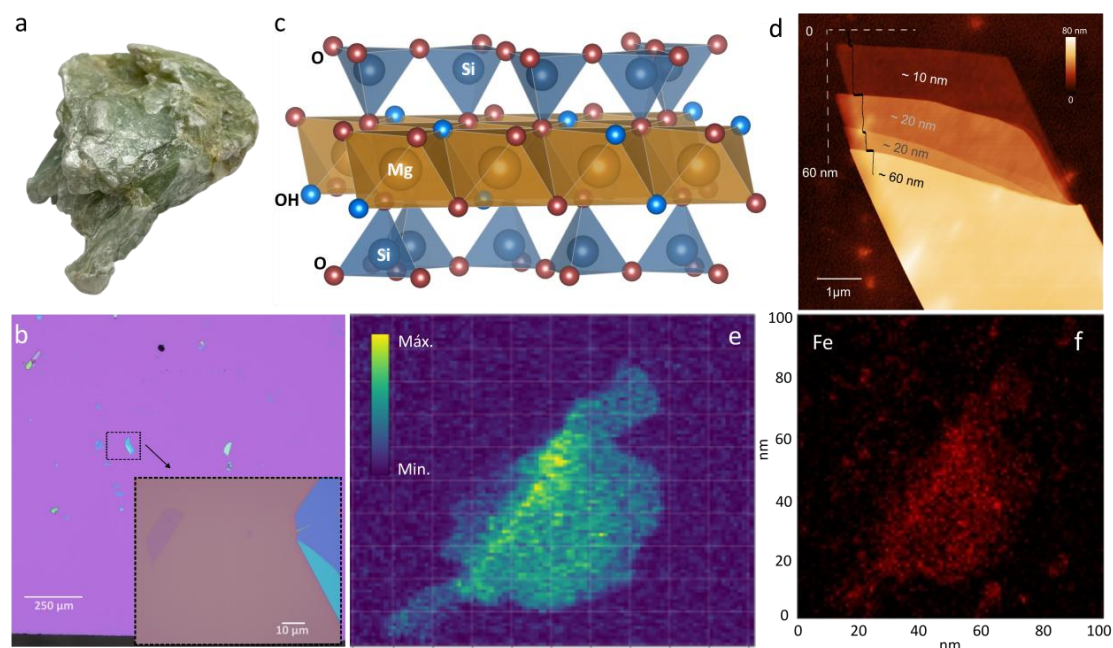


Figure 1: (a) Natural talc crystal. (b) Optical microscopy image of talc flake on SiO_2/Si substrate. (c) Talc crystalline structure (T–O–T), consisting of two SiO_4 tetrahedral layers sandwiching an octahedral $\text{MgO}_4(\text{OH})_2$ layer, forming the characteristic 2:1 phyllosilicate structure. (d) AFM topography image showing thickness steps of the exfoliated flake. (e) Nano-XRF map of a talc flake showing the total fluorescence intensity. (f) Spatial distribution of Fe within the flake.

Improvement of radiation resistance of GaAs solar cell with InGaAs/GaAsP quantum wells

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The introduction of a multi-quantum well (MQW) structure into gallium arsenide (GaAs) solar cells as shown in Fig. 1(a) enables effective broadening of the spectral response range, which in turn significantly enhances the short-circuit current density (Jsc). This structure has emerged as one of the most promising technical routes in the field of next-generation photovoltaic technologies. Under electron irradiation conditions with an energy of 1 MeV and a fluence of $1 \times 10^{15} \text{ cm}^{-2}$, the radiation resistance of quantum well solar cells (QWSCs) is notably inferior to that of the GaAs solar cells without the MQW structure. It is believed that radiation induces crystal defects within the forbidden gap, forming trap states that localize free carriers, resulting in the so-called Carrier Removal (CR). The CR effect brings about a significant transformation of the intrinsic region (i-region), leading to n-type doping behavior and ultimately resulting in the collapse of the built-in electric field within the depletion layer. This effect is particularly pronounced in MQW structures with a thick intrinsic region. In this study, the influence of intentional doping in the MQW region and the position of the MQW within the P-type base region (Fig. 1(b) and (c)), on the radiation resistance of QWSCs was systematically investigated. The results demonstrate that mild intentional doping in the quantum well (QW) region and locating the QW away from the emitter can enhance the irradiation resistance of QWSCs, with the retention coefficient of the short-circuit current density (Jsc) and fill factor (FF) increased by more than 30% after irradiation, thereby significantly mitigating the degradation of the cell's photoelectric conversion efficiency. This study provides a feasible technical strategy for optimizing the radiation resistance of MQW-based GaAs solar cells.

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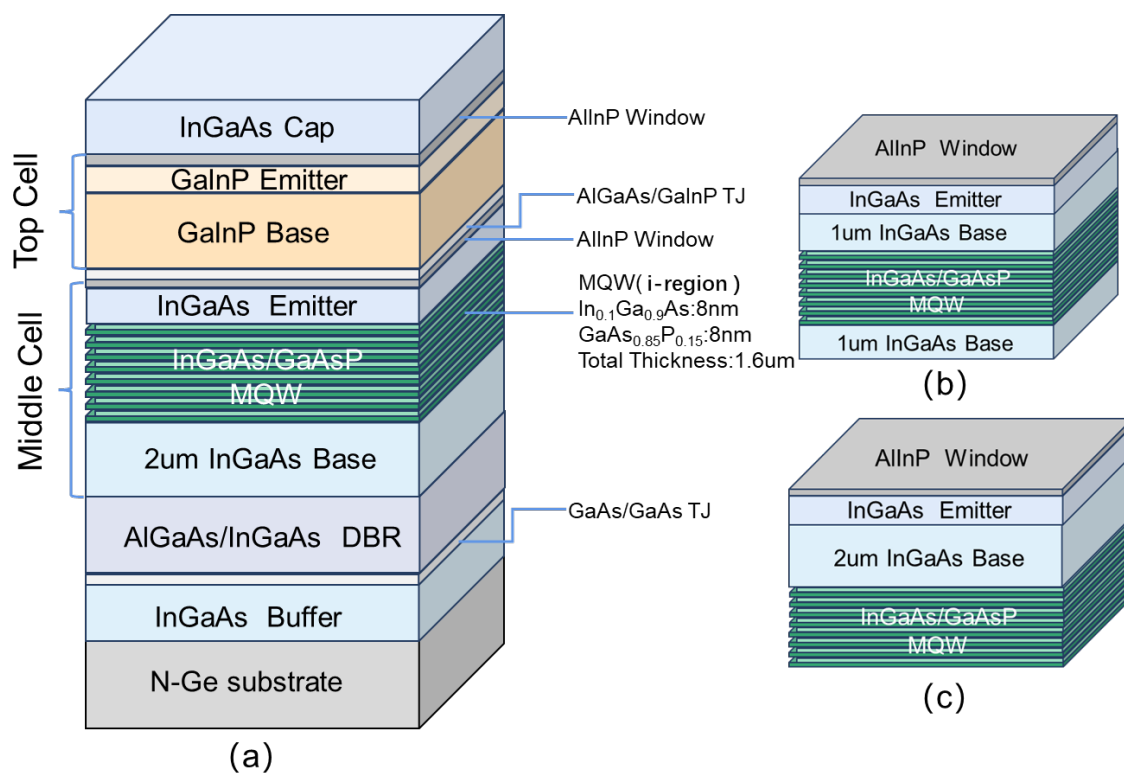
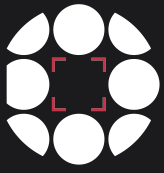


Figure 1: (a) Schematic structure of a lattice matched GaInP/InGaAs/Ge TJ solar cell with InGaAs/GaAsP QWs. (b) and (c) Schematic structure of the position of MQW in P-type base region of the middle cell.



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