50 years of the Institute of High Pressure Physics Polish Academy of Sciences
Highlights in III-V semiconductors, THz physics and nanomaterials
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# Mechanism of thermal degradation of InGaN

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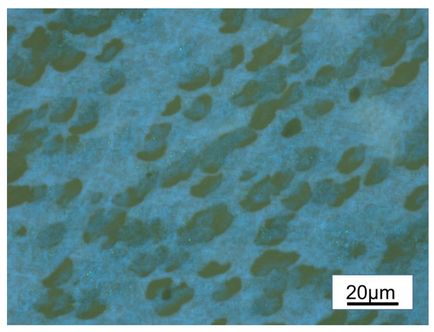
## Motivation

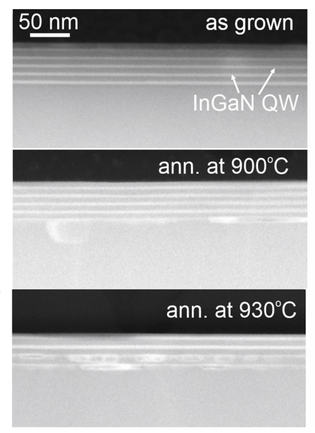
- InGaN layers tend to degrade into voids and high In-content phases when exposed to temperatures higher than the growth temperature. It may happen during MOVPE growth of p-type layers, which are grown at temperature around 200 degrees higher than InGaN quantum wells (QWs).
- The temperature affecting InGaN layers is decreasing with increasing In content.

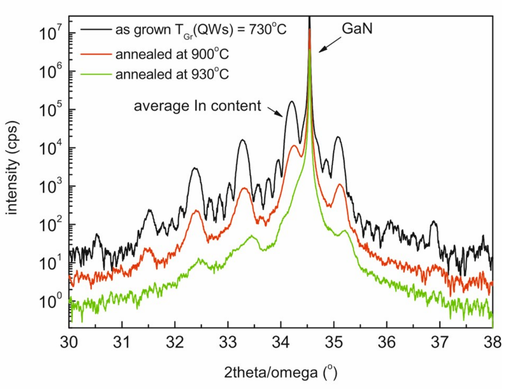



Fluorescence image of a structure with $In_{0.18}Ga_{0.72}N$ QWs, areas of lower intensity contain degraded QWs

## TEM and XRD

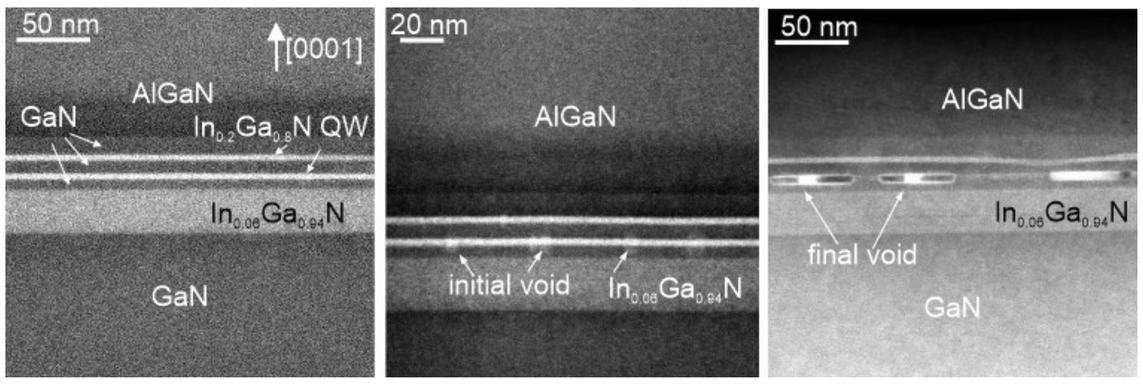
The thermal degradation is typically initiated in the first grown quantum well and then, with increasing temperature or annealing time, affects subsequent InGaN quantum wells.

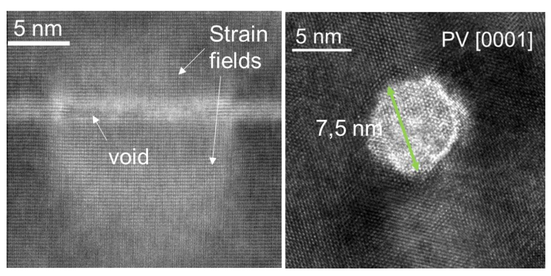



## Initial and final voids

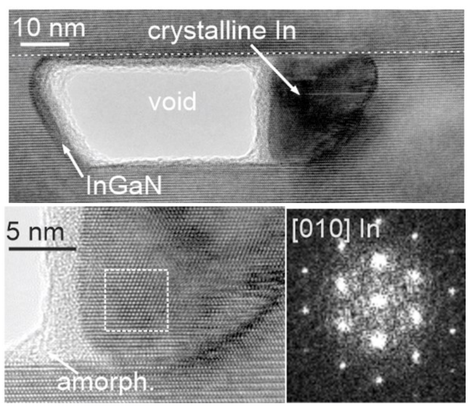
There are three various areas observed in TEM studies: left– undestroyed structure, middle –InGaN QWs with few nm size voids (initial), right– degraded lower QW into voids filled with In-rich phases.

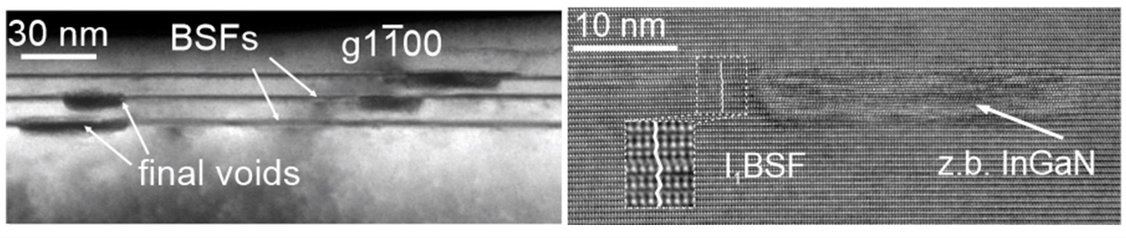


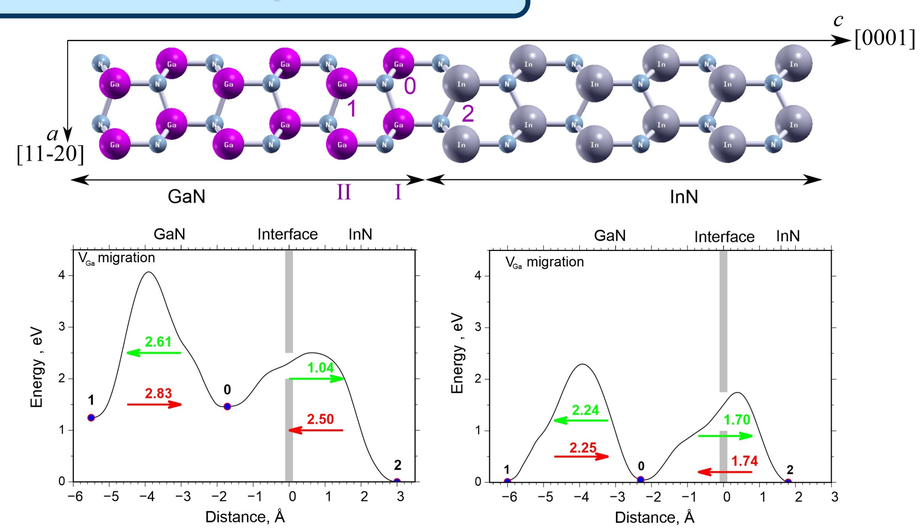

**Initial voids** have few nm diameter and are located at the lower interface with GaN. The characteristic feature is the strain field surrounding the voids visible in STEM studies.

**Final voids** are a few tens of nm in diameter and are aligned with the upper interface of the former QW. The voids are typically surrounded by a frame of high In -content InGaN and may contain a precipitation of crystalline In and some amorphous material inside. The voids are attached to extended basal stacking faults (BSF) located at the upper interface with GaN.




## DFT studies of vacancy diffusion

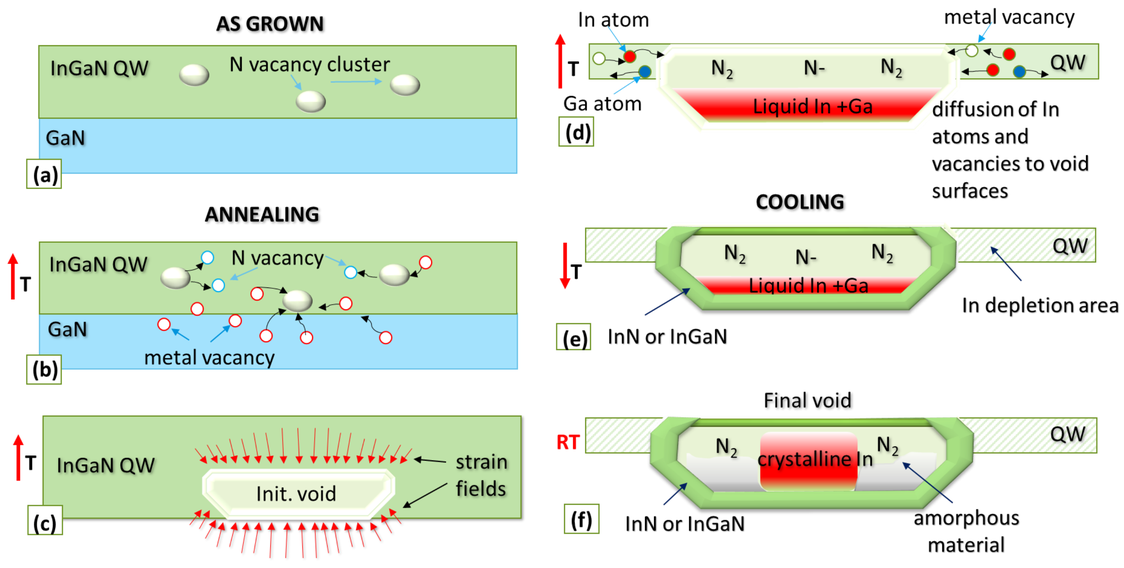



Strained InN/GaN interface

Relaxed InN/GaN interface

DFT calculations show that there is a lower energy barrier for gallium vacancy migration across the strained InN/GaN interface. Moreover, gallium vacancies are more mobile than nitrogen vacancies. Indium vacancies are most mobile in the lateral direction in the vicinity of the InN/GaN interafce.

## Mechanism of thermal degradation




## References

1. J. Smalc-Koziorowska et al., *Role of Metal Vacancies in the Mechanism of Thermal Degradation of InGaN Quantum Wells*, ACS Appl Mater Interfaces, 13, 7476 (2021).
2. R. Hrytsak, et al. *DFT study on point defects migration through the pseudomorphic and lattice-matched InN/GaN interfaces*, Computat. Mater. Sci., 186, 110039 (2021).
3. A. Lachowski et al. *Improving thermal stability of InGaN quantum wells by doping of GaN barrier layers*, J. of Alloys and Compounds 900, 163519 (2022).
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## Summary

- The heat treatment of $In_xGa_{1-x}N$ QWs during post-growth annealing or during overgrowth by high-temperature layers leads to their structural degradation;
- First structural changes inside the $In_xGa_{1-x}N$ QWs are manifested by formation of <10 nm diameter hexagonal shaped initial voids which increase in sizes upon prolonged annealing;
- Larger voids (>>10nm) found in the degraded areas contain In-rich phases, while the QW between the voids contain highly reduced amount of In;
- In case of the $In_xGa_{1-x}N$ QWs deposited on undoped GaN, the degradation starts in the first QW and then sequentially occurs in the following QWs;

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