# A puzzle in understanding the discrepancy between theory and experiment in In(Ga)N/GaN short period superlattices

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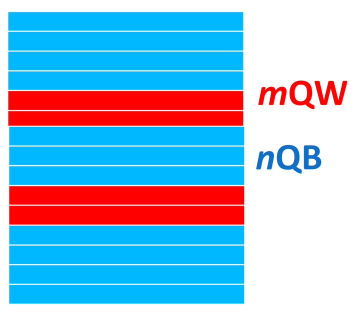
## Early attempts to grow Short Period InN/GaN Superlattices

Modern nitride light emitters of visible and UV light are based on Quantum Wells (QWs) and Superlattices (SLs) of (InAlGa)N/GaN.
SLs are structures of altenative sequences of quantum wells (QW) and quantum barriers (QB), where band gaps $E_g$ fulfill:

$E_g(QW) < E_g(QB)$;




Notation: QW/QB or *m*QW/*n*QB, where: *m*, *n* = number of atomic monolayers. In InGaN/GaN **Short Period SLs**- *m*, *n* < 7.

Pioneering work of A. Yoshikawa et al. [1] proposed the concept of binary SPSL ***m*InN/*n*GaN** with the purpose of avoiding difficulties with growth of $In_xGa_{1-x}N$ with x>0.3 %. This limitation blocked getting devices with wavelength above around 500nm.

**There was the common believe that the SPSLs grown accordingly represent a combnation of binary alloys mInN/nGaN**

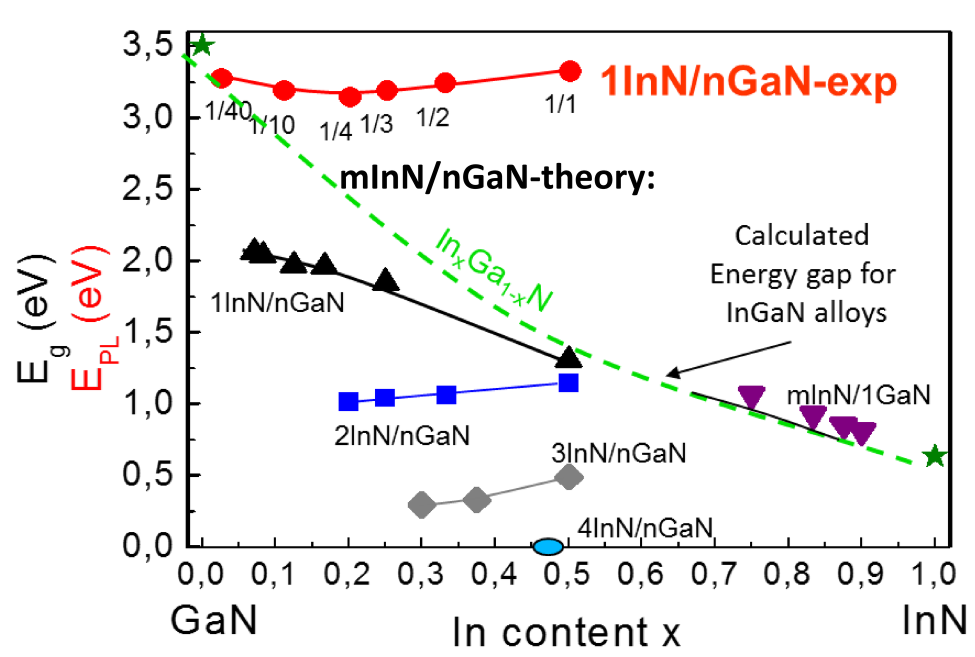
## Predicted advantages of nitride Short Period Superlattices

- Precise tuning of the band gap $-E_g$ value (emission wavelength) by changes of the layers numer *m and n*. It was predicted that in *m*InN/*n*GaN SPSLs energy gap can change by more than 3eV. Down to 0 eV.
- Band-gap closing.
- Substantial reduction in the number of "nonradiative" defects caused by the lattice mismatch
- More uniform band-filling of all QWs of SPSLs compared to „standard" QWs - carrier tunneling between QWs through narrow barriers.
- Stable emission wavelength with the increasing the driving current. The related emmiters with narrow QWs and QBs are less sensitive to screening of the built-in electric field [2].

## Discrepancy between experimental results and theory

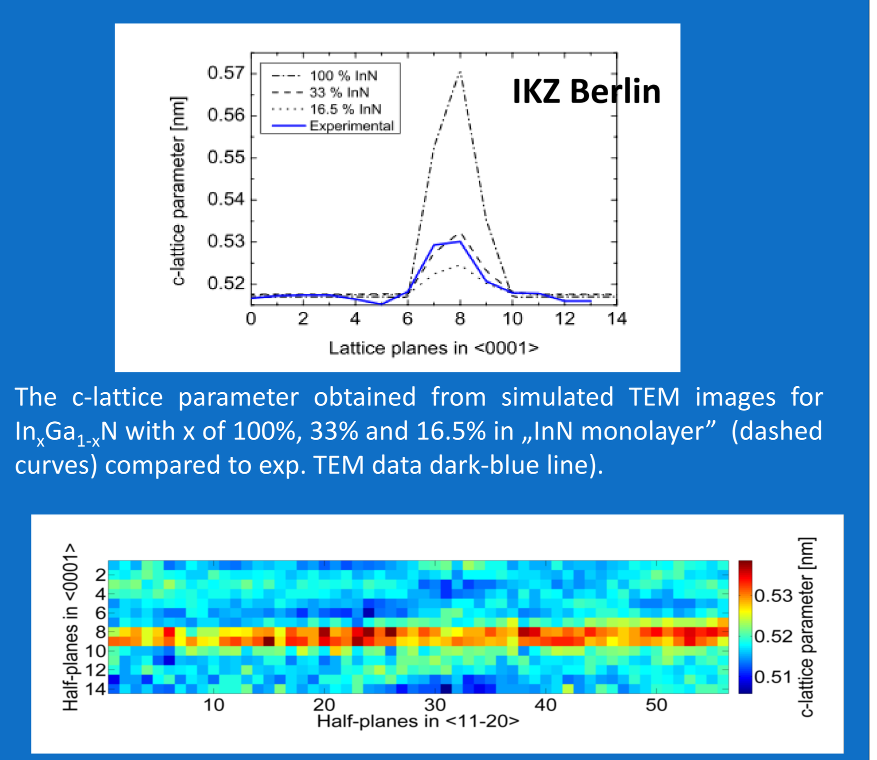
Obtained in our Institute experimental and theoretical results as well as results from other research groups showed strong discrepancy between experiment (photoluminescence, $E_{PL}$) and theoretical calculations of the band gap.

PL energies in InN/GaN SLs - experiment vs. theory




Explanation
T. Suski, et. al. [2]

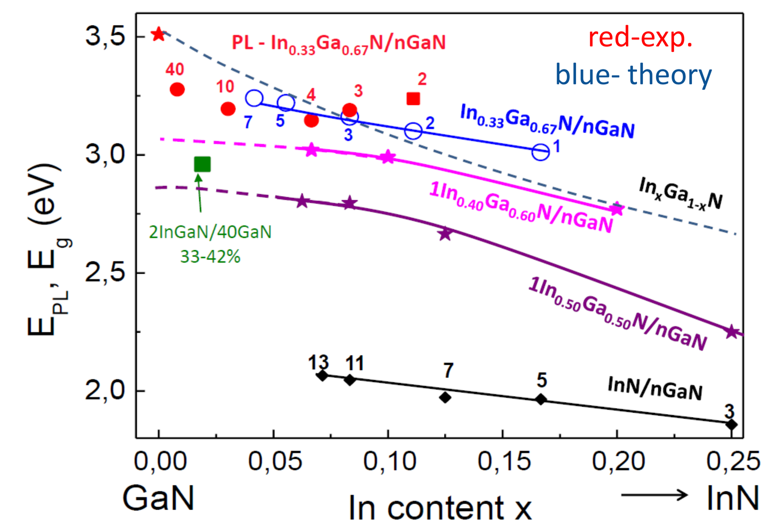
Quantitative high resolution transmission electron microscopy studies of intentionaly grown 1InN/10GaN short-period SPL [3]



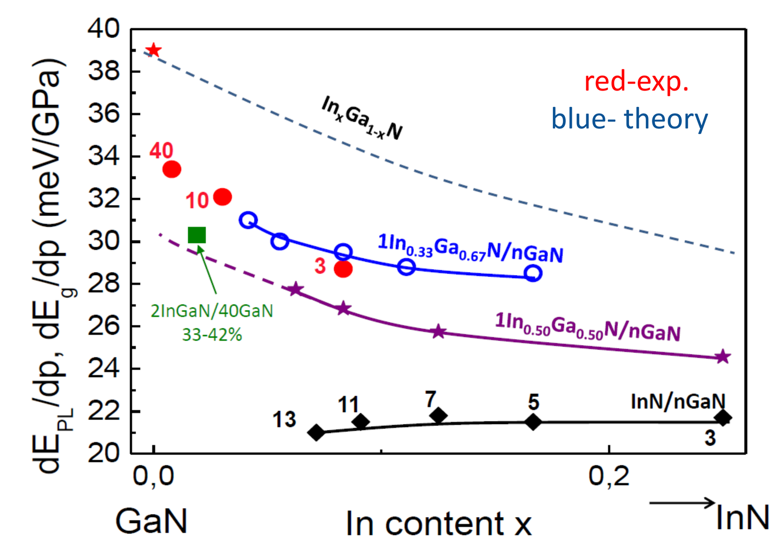

The c-lattice parameter obtained from simulated TEM images for $In_xGa_{1-x}N$ with x of 100%, 33% and 16.5% in „InN monolayer" (dashed curves) compared to exp. TEM data dark-blue line).

*Local c-lattice parameter map in the region of the QW monolayer.*

Close similarity of the calculated band-gap with **PL Energy** of $In_{0.33}Ga_{0.67}N$ SPSLs [2]




Close similarity of the calculated band-gap pressure coeff. with **Pressure shift of PL energy** [2]




The same as above, but for pressure coefficients

**$E_{PL}$ of 1InN/nGaN is much higher than calculated $E_g$**

**TEM studies revealed $In_xGa_{1-x}N$/GaN Superlattice with x=0.33 instead of InN/GaN !!!**

**Good agreement between theory and experiment for 33% of In!**

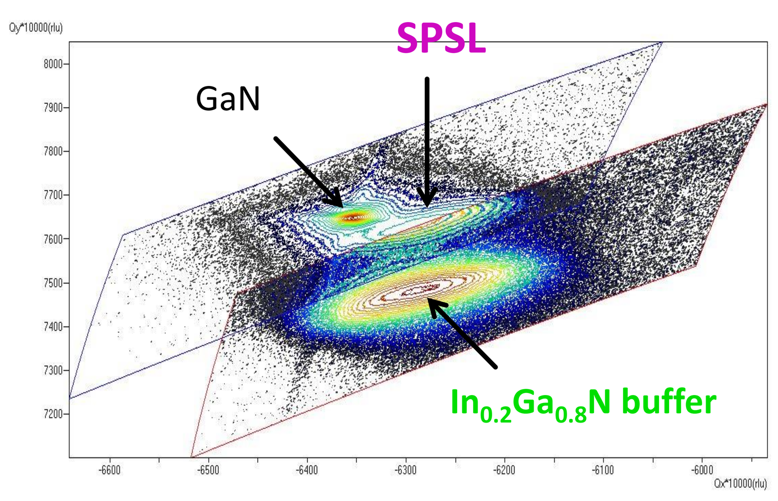
## Possible Solution to obtain higher $E_{PL}$: Superlattice grown on relaxed InGaN buffer

**Due to limitations in InN/GaN growth other ways of to get lower $E_g$ are nrcessary [4,5]**

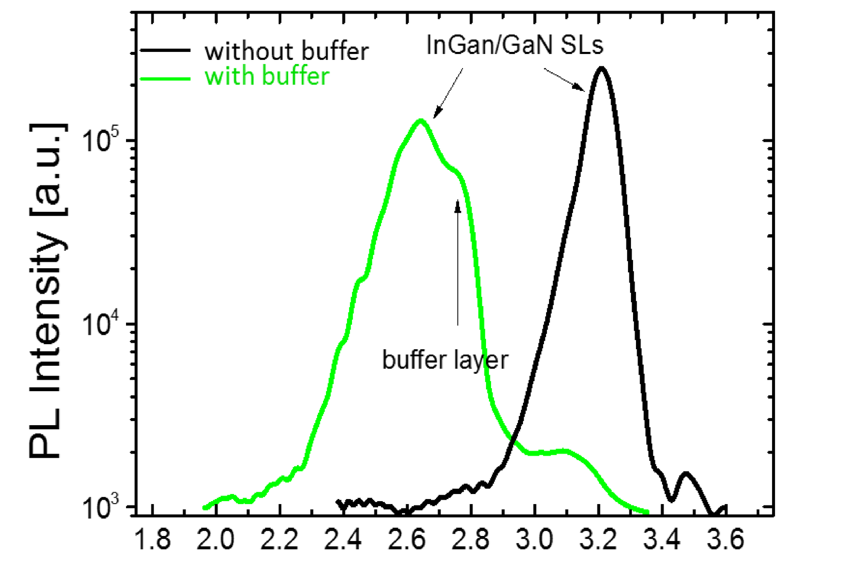
Example: MOVPE growth of Short Period Superlattices $2In_{0.20}Ga_{0.00}N$/ 40GaN on relaxed (thick) $In_{0.17}Ga_{0.83}N$ buffer

**Positive proof of the concept**

Introducing InGaN buffer layer leads to record energy shift of 580 meV (3.21 - 2.63 eV) – resulting from decrease of mismatch between QW and QB layers.




Reciprocal space map n InGaN/GaN SPSL on InGaN buffer substrate – SLs strucutre strained to InGaN buffer layer.




Photoluminescence studies comparison of SPSLs without and with buffer layer

## Summary

- Our studies found an explanation of dicscepency observed between experiment and theory: **instead of intended InN monolayer in QW of SPSl, $In_{0.33}Ga_{0.67}N$ monolayer was grown and examined in variety of previously studied materials.**
- Performed theoretical calculationS are in good agreement with $In_{0.33}Ga_{0.67}N$/GaN SLs case.
- High pressure studies confirm additionally theoretical calculations and HRTEM results.
- Problem of high In-content (higher than 33%) superlattices is still unsolved.
- The idea of using SPSL with QWs matched to thick InGaN „buffer" instead of GaN seems to work well.

## References

[1] A. Yoshikawa et al. Appl. Phys. Lett., 90, 073101 (2007).
[2] I. Gorczyca et al.. Review paper:
[3] T. Suski et al. Appl. Phys. Lett. 104, 182103 (2014).
[4] A. Duff et al. Phys. Rev. B, 89 (085307 (2014).
[5] M.Siekacz et al. Superlattices and Microstructures, 133, 106209 (2019)

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