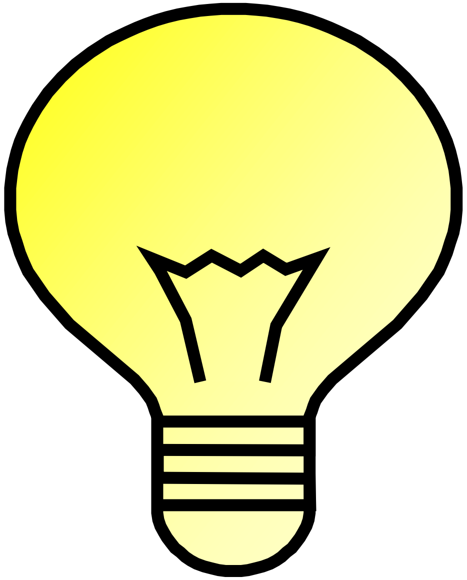
Simulation tools for design of advanced LEDs and modeling of related technologies



STR Group

www.str-soft.com

Outline

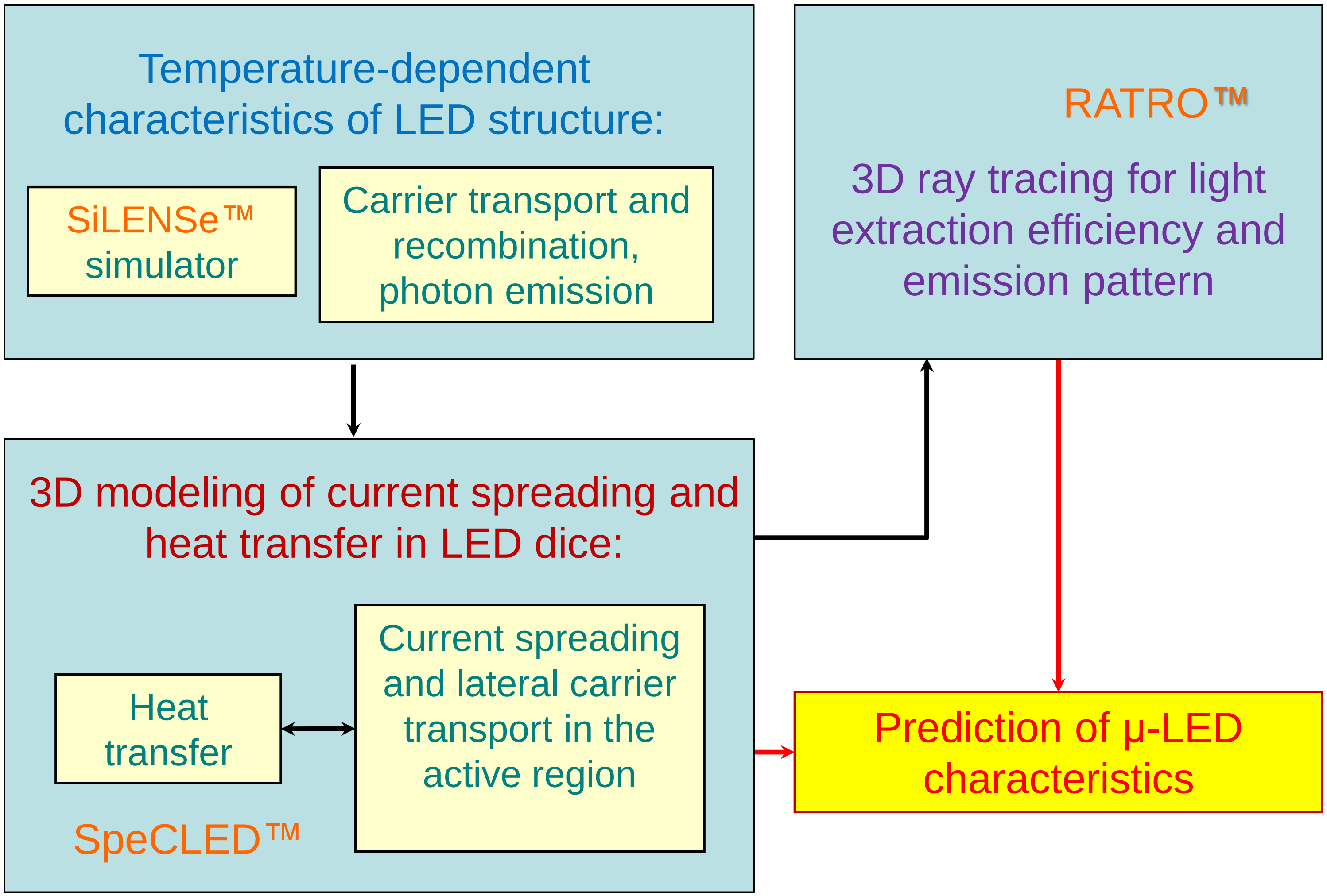
- Software package for design and optimization of advanced LEDs. SimuLED™ software package
- Optical and Thermal Management of LED Lamps. SimuLAMP™ software package
- Growth of Group-III nitrides by MOCVD. Virtual Reactor™ Nitride Edition
- Modeling of the characteristics of III-Nitride device heterostructures grown by MOCVD. STREEM™-InGaN software
- Stress and dislocation behavior and wafer bowing in GaN growth on Silicon. STREEM™-AlGaN software
- Growth of GaN by HVPE. Hydride Epitaxial GaN Simulator (HEpiGaNS™) or VR HVPE

Software package for design and optimization of advanced LEDs

SimuLED™ software package

SimuLED™ package

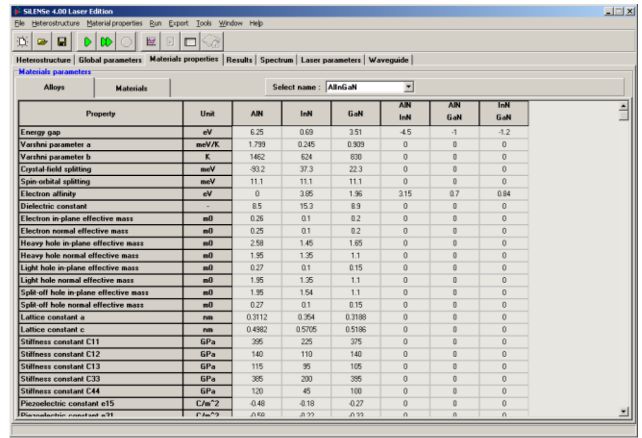
https://www.str-soft.com/devices/simuled



SiLENSe™: module for designing of LED/LD heterostructure

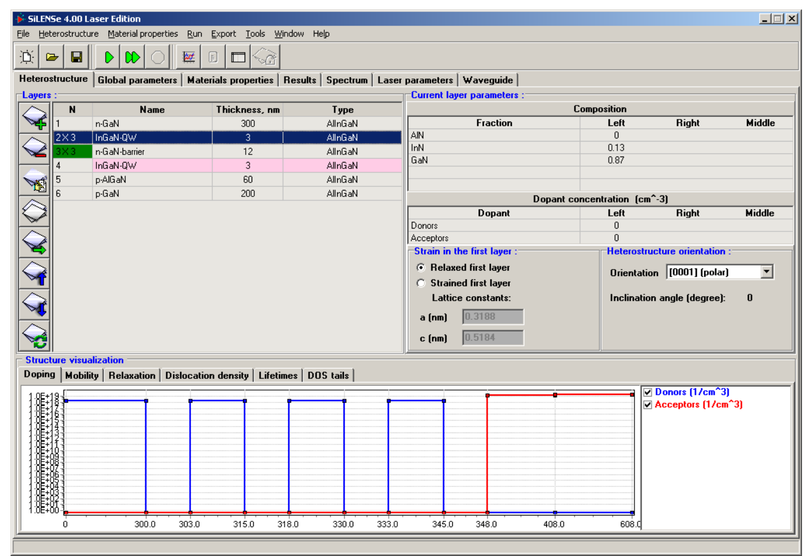
SiLENSe™ input parameters

- ✓ Number of layers
- ✓ Layer thickness
- ✓ Layer composition (including graded composition)
- ✓ Polar, non-polar, and semi-polar orientations
- ✓ Layer doping
- ✓ Layer degree of relaxation
- ✓ Temperature
- ✓ Dislocation density



Materials database

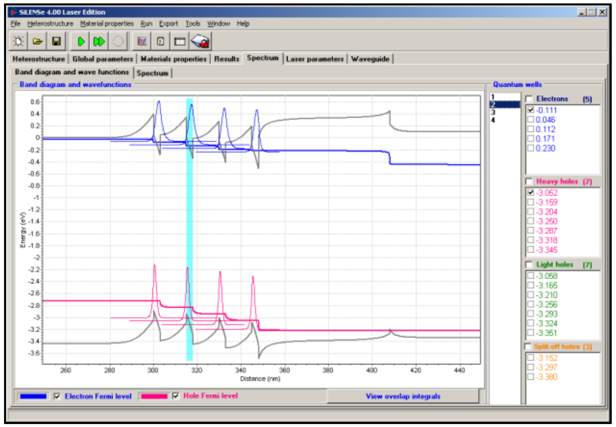
Structure specification

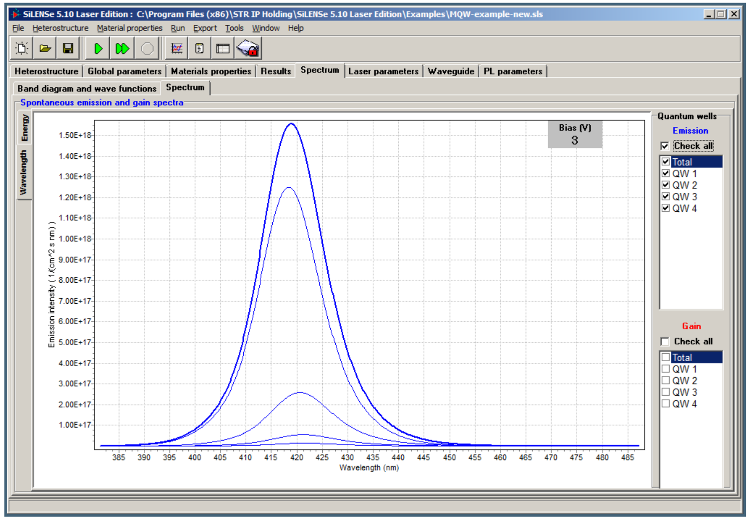


SiLENSe™: module for designing of LED heterostructure

Parameters computed with SiLENSe™

- ✓ Band diagram and electric field
- ✓ Carrier concentrations
- ✓ Carrier fluxes and leakage
- ✓ R_{rad}, R_{SRH}, R_{Auger} → IQE
- ✓ Energy levels in QWs
- ✓ Emission and gain spectra
- ✓ Simulation of optical excitation (PL)

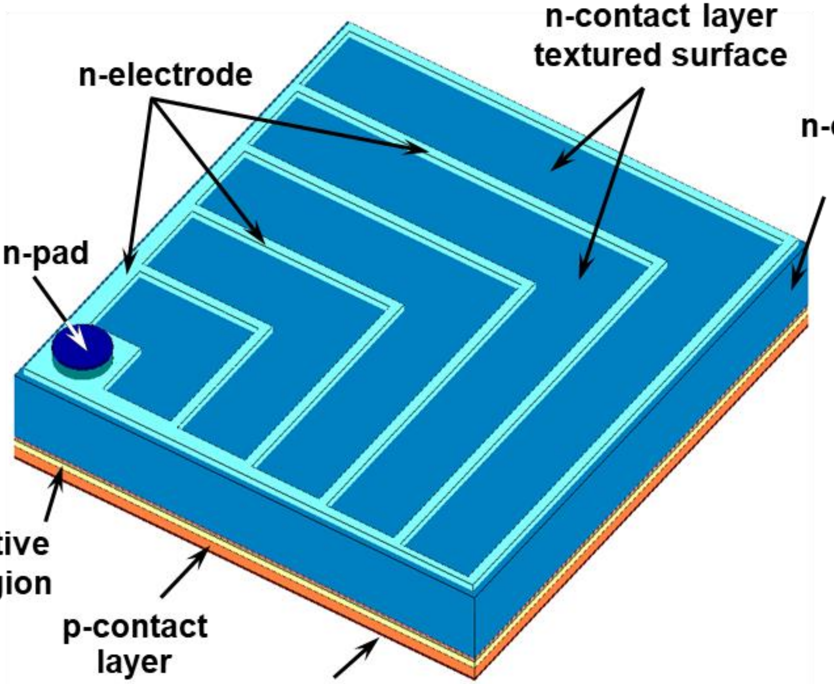




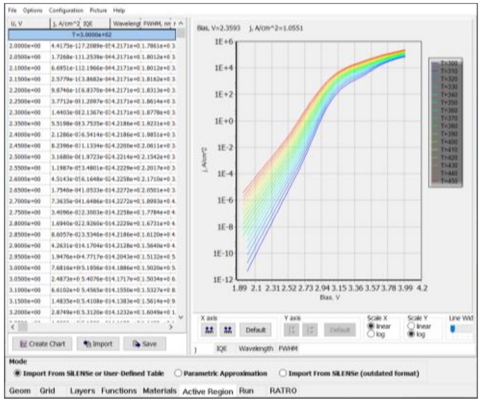
SpeCLED™: current spreading and heat transfer

SpeCLED™ input parameters

- ✓ Chip design
- ✓ Material properties
- ✓ Surface passivation
- ✓ Heat sink specification
- ✓ Forward current
- ✓ Characteristics of active region: $j(U_b,T)$, $IQE(U_b,T)$



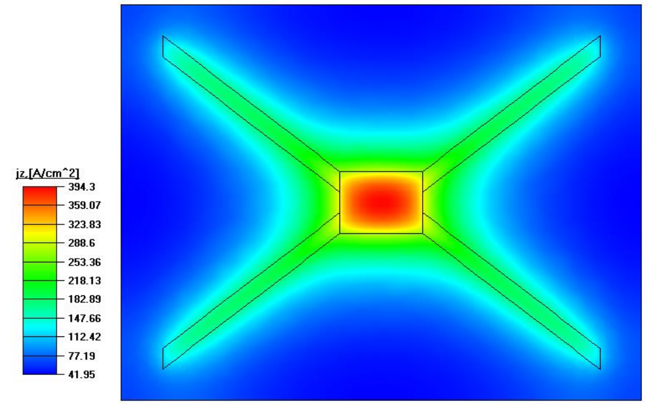
Characteristics of active region calculated by SiLENSe™ can be used as input for SpeCLED™

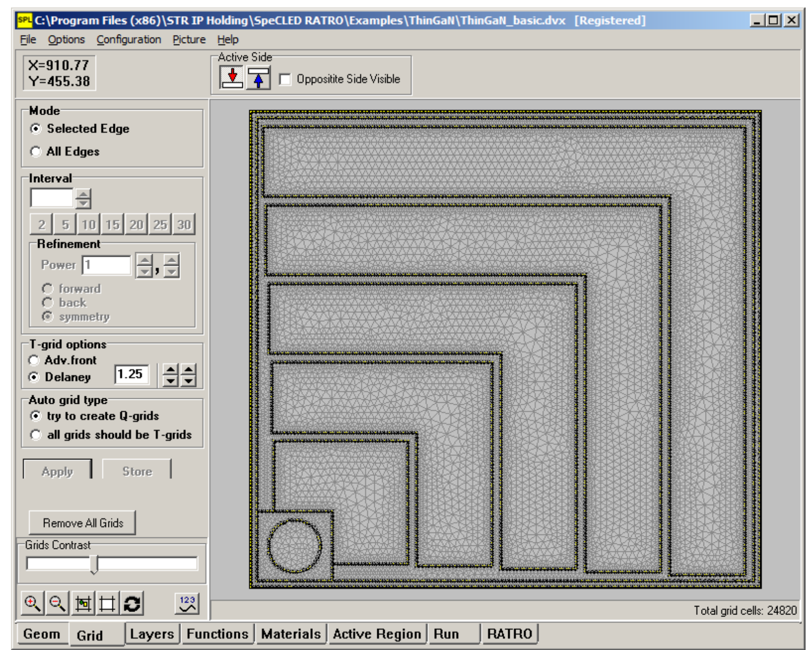


SpeCLED™: current spreading and heat transfer

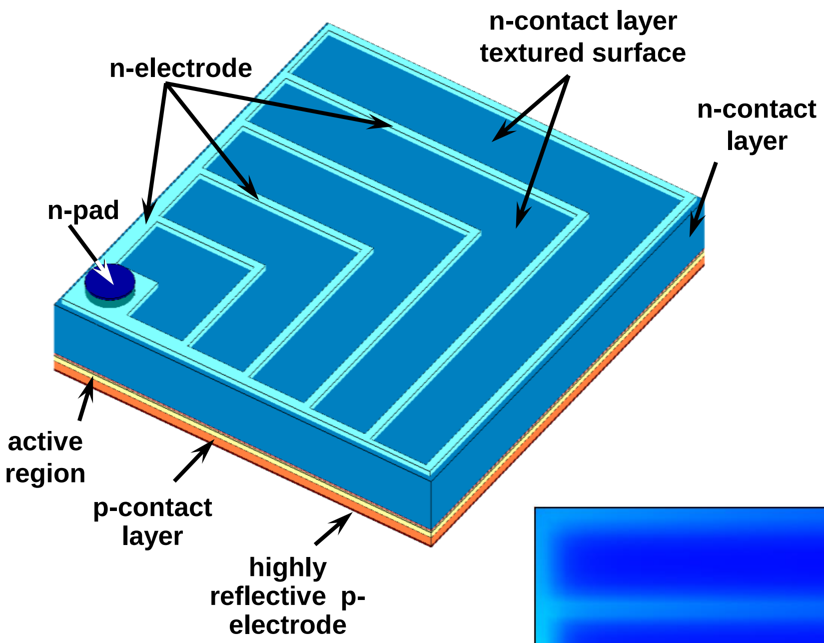
Parameters computed with SpeCLED™

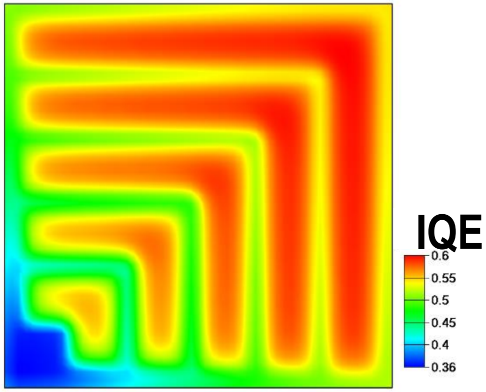
- ✓ 3D distributions of the electric potential, current density, and temperature in the whole die
- ✓ 2D distributions of the p-n junction bias, current density, IQE, and temperature in the active region plane
- ✓ I-V characteristic
- ✓ Series resistance
- ✓ EQE and WPE





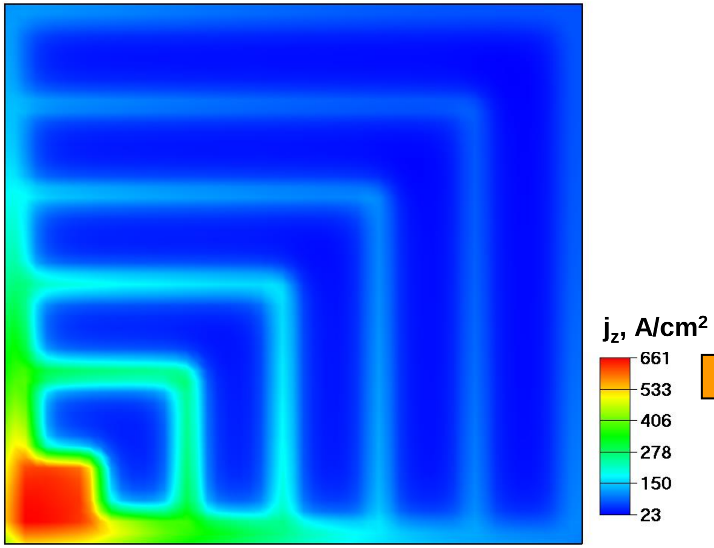
SpeCLED™/RATRO™ coupling





$$W = \frac{j_z(x,y)}{q} \cdot \hbar\omega \cdot \eta_{int}(x,y)$$

Non-uniform distribution of light emission from the active region



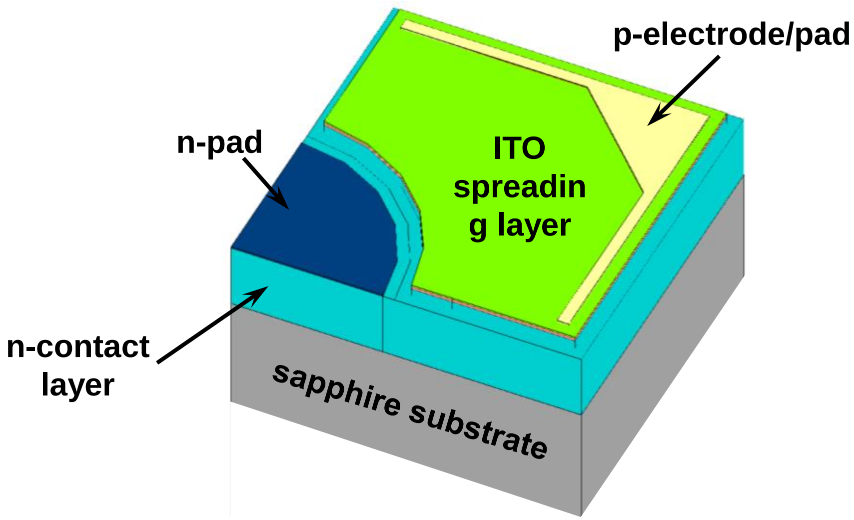
SpeCLED™ computations

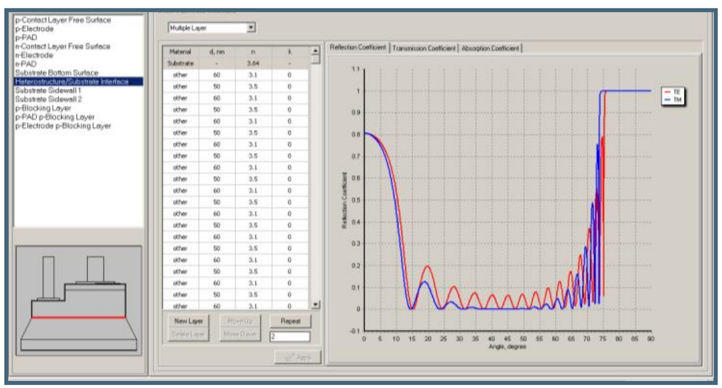
RATRO™

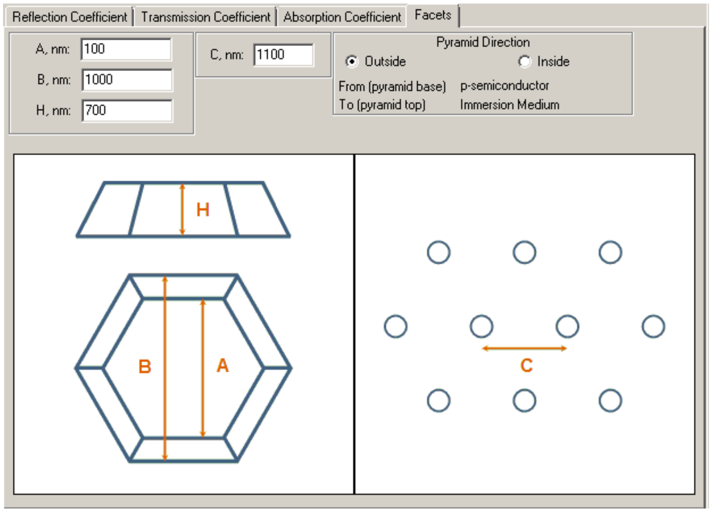
RATRO™: Analysis of optical characteristics of LED dice

RATRO™ input parameters

- ✓ Chip design
- ✓ Bulk optical properties
- ✓ Surface optical properties
  - ✓ Mirrors
  - ✓ Multiple layer coatings
  - ✓ Surface patterning
  - ✓ DBRs

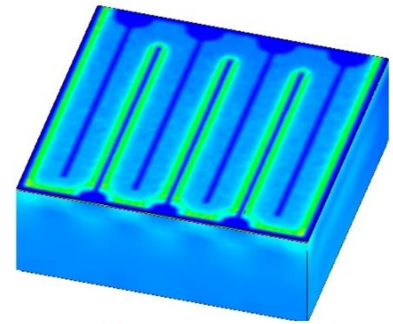




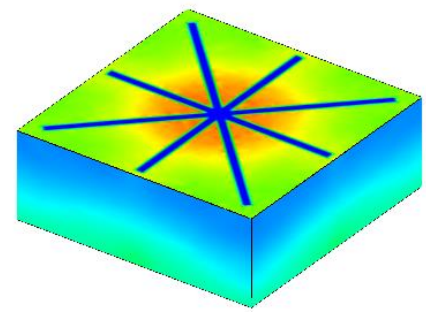


RATRO™: 3D ray-tracing analysis of optical characteristics of LED dice

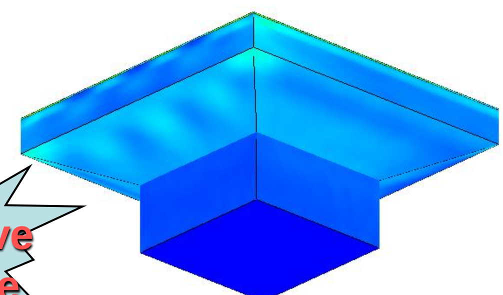
RATRO™ capabilities and computed parameters



- ✓ The effective reflection, absorption and transmission coefficients of n- and p- electrodes are calculated by the program accounting for the interference in the multilayer contact
- ✓ Patterned surfaces are supported



- ✓ Light extraction efficiency from an LED die is predicted
- ✓ Far-field and near-field emission patterns
- ✓ Light polarization distribution
- ✓ Various die configurations, including shaped substrate are supported



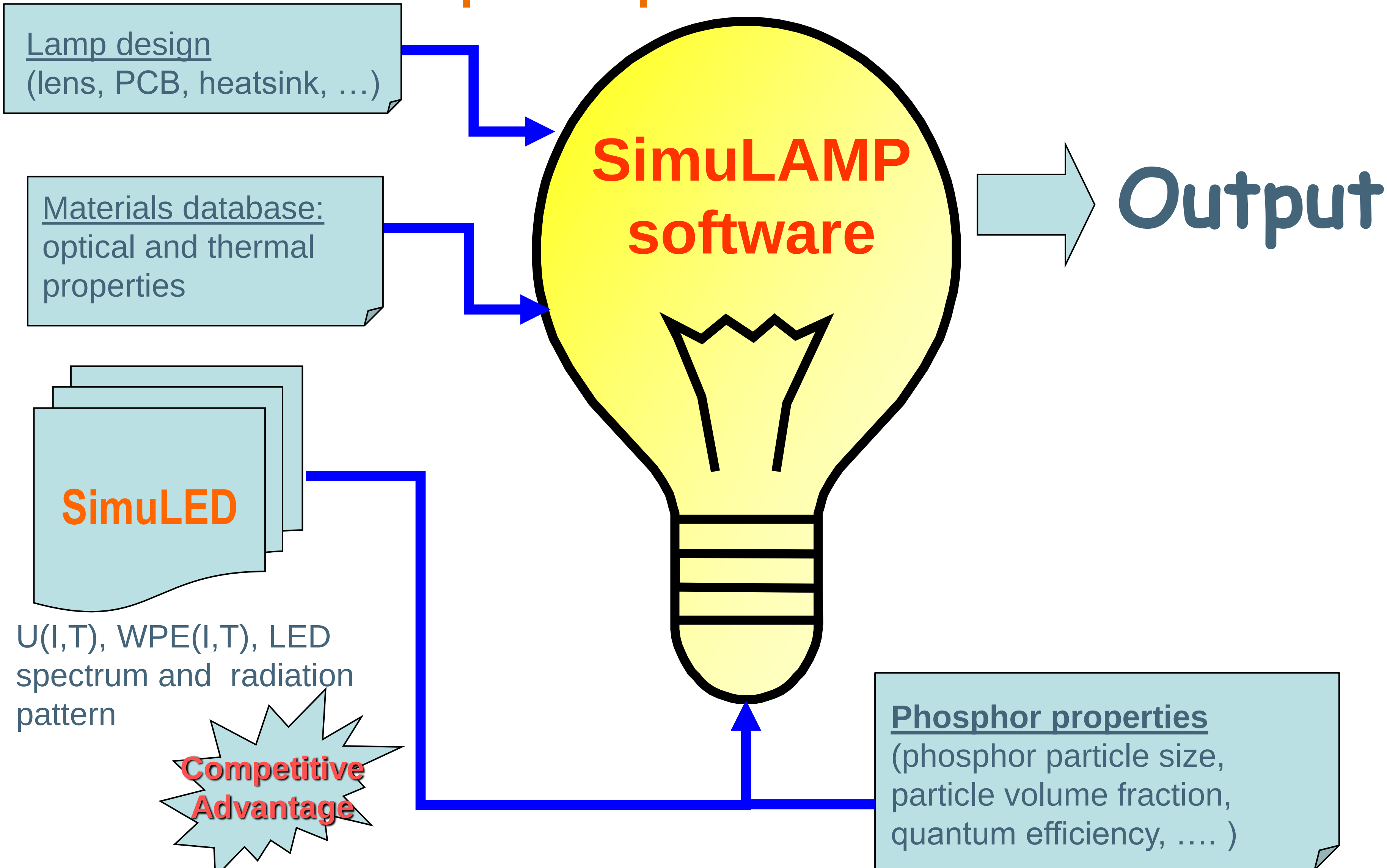
- ✓ Consideration of non-uniform electroluminescence intensity distribution over the active region plane

Competitive Advantage

Optical and Thermal Management of LED Lamps

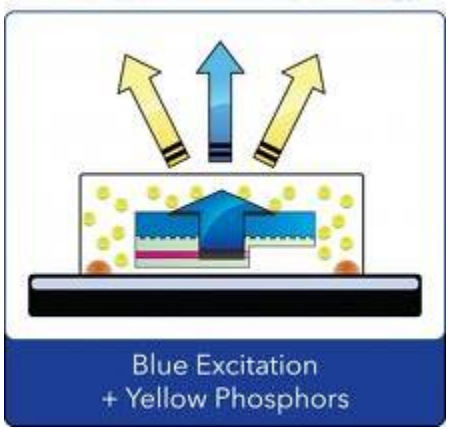
SimuLAMP™ software package

Input/Output data in SimuLAMP software



Output from SimuLAMP™ modeling

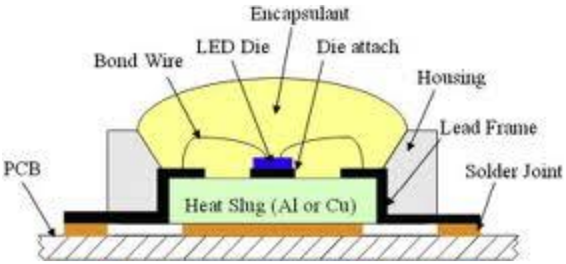
- Solution of coupled optical/thermal problem in a complex package geometry accounting for heat release in the LED chip and heat release in an encapsulant due to light absorption and Stokes shift



- Advanced model of light conversion in individual phosphor and phosphor mixtures (for white-light LED lamps)

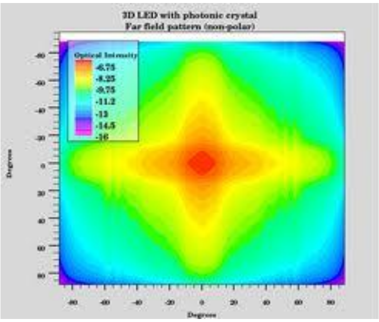
- Support of single- and multichip package configurations including RGB LEDs

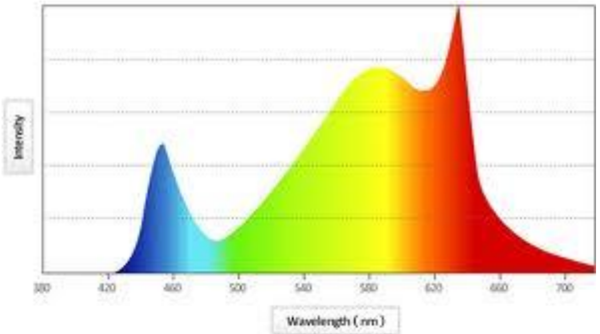
- Simulations of the electrical circuit used in operation of multi-pixel LED array



- Analysis of package operating in DC/AC/Quasi-CW modes

Characteristics of LED lamps predicted by SimuLAMP





- Temperature distribution over the LED package, thermal resistance
- Near-field and far-field radiation patterns
- Output light spectrum, color uniformity
- Optical losses in the package
- CRI, CCT and other characteristics of white-light LEDs

Growth of Group-III nitrides by MOCVD

Virtual Reactor Nitride Edition

Modeling approach

Input parameters:

- Reactor geometry
- Operating temperature and pressure
- Gas flow rates

Available precursor gases:

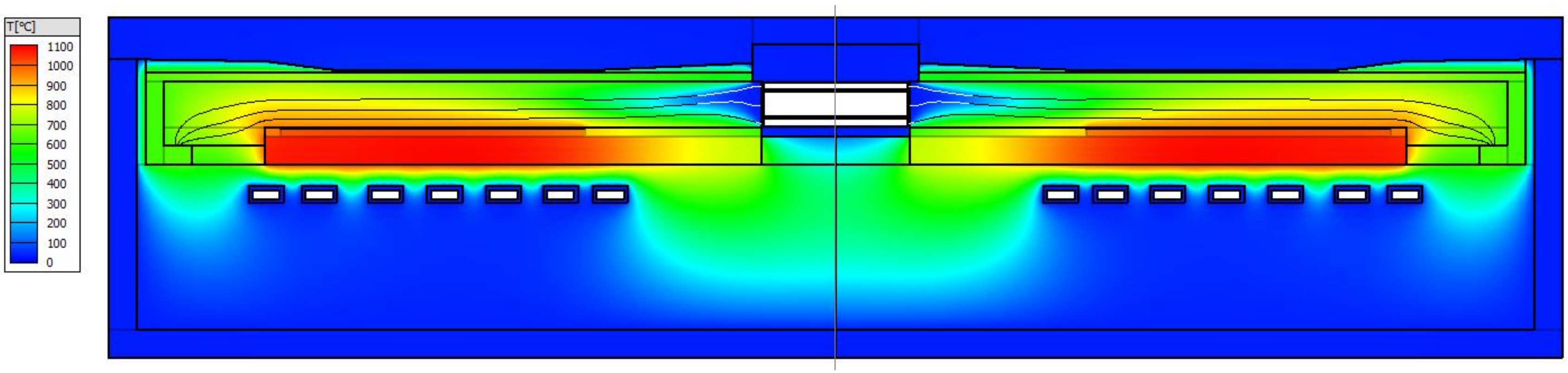
- MO source: TMGa, TEGa, TMAl, TMIn
- Carrier gas: NH_3, N_2, H_2
- Dopant source: SiH_4, $MgCp_2$

Modeling of MOCVD growth of the following materials:

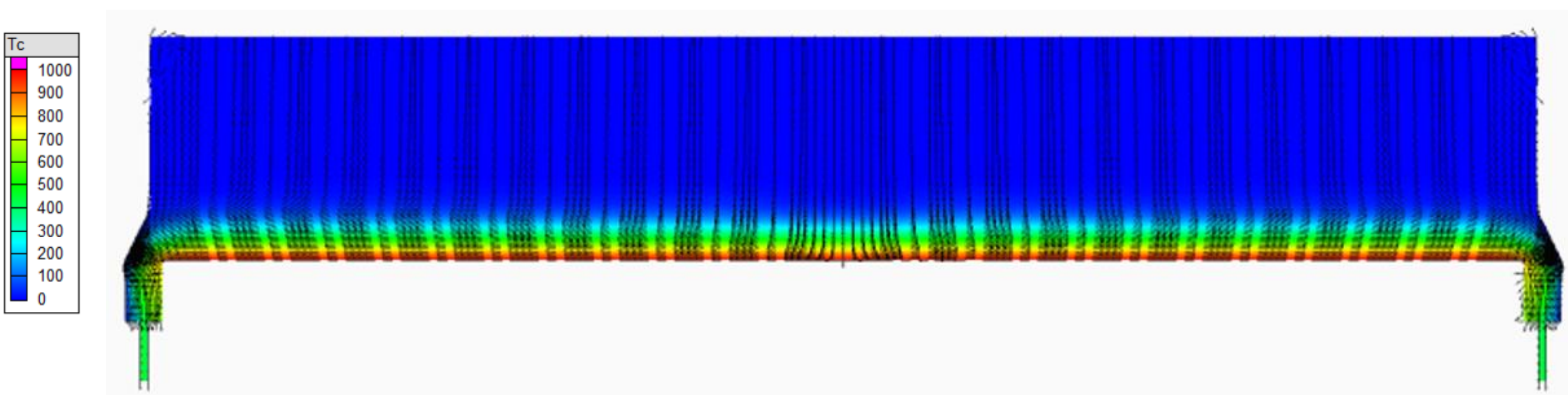
- GaN
- AlN
- AlGaN
- InGaN
- InAlN

Reactor geometry and temperature

Planetary reactor



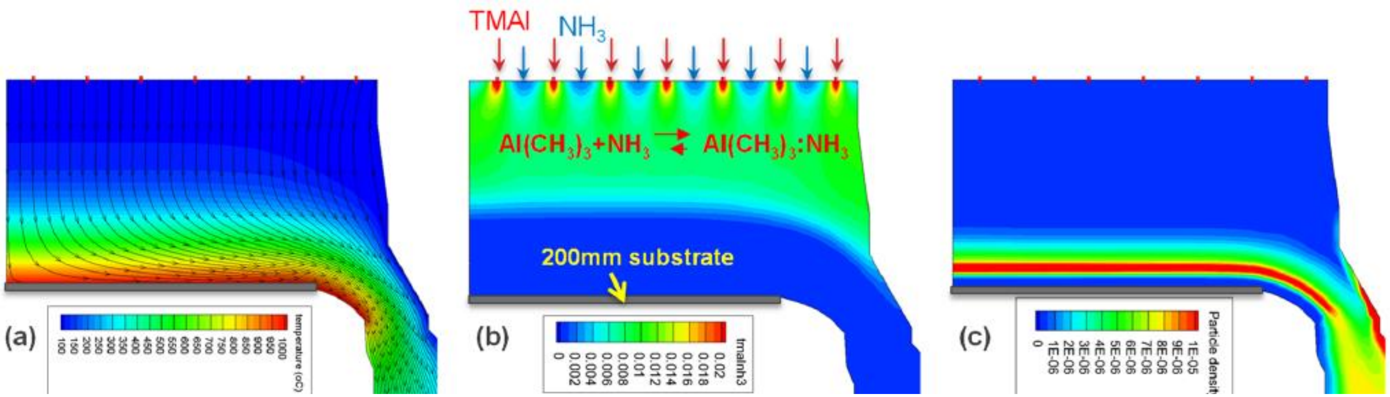
Rotating disk reactor



Growth of the AlGaN/GaN HEMT Structure in Veeco's Propel™ reactor

Process Condition Optimization for High Throughput and High Efficiency Growth of the AlGaN/GaN HEMT Structure in a Single Wafer Rotating Disc MOCVD Reactor

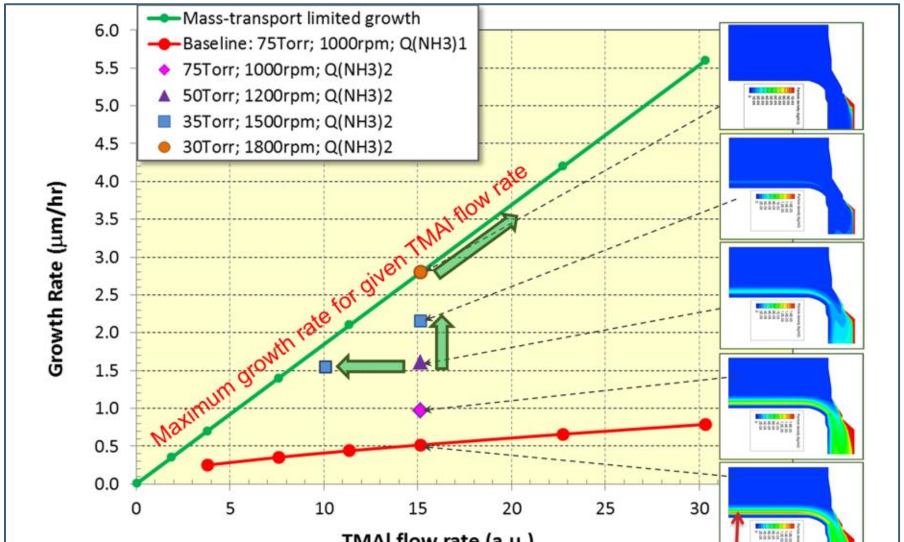
B. Mitrovic*, R Bubber, J. Su, E. Marcelo, M. Deshpande, and A. Paranjpe



Optimization of the process conditions allows elimination of parasitic reactions

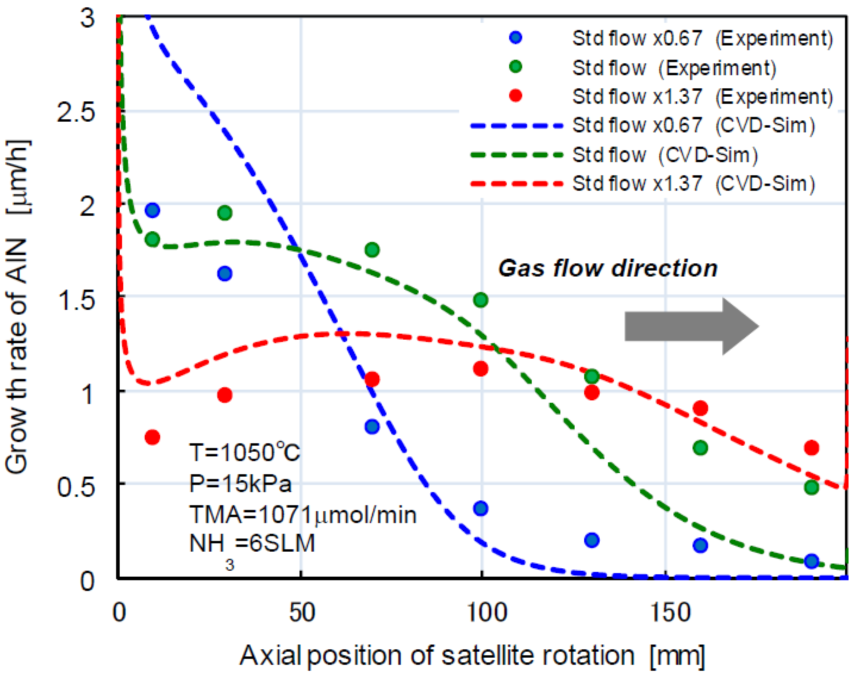
Contours based on CFD and chemistry modeling: (a) Temperature and streamlines, (b) adducts (TMAl:NH3) mass fraction, (c) particle density (kg/m3)

Significant improvement in process time (~50%) and source efficiency is achieved during AlN/AlGaN superlattice HEMT structure growth on 200mm Si substrate while maintaining the desired material quality

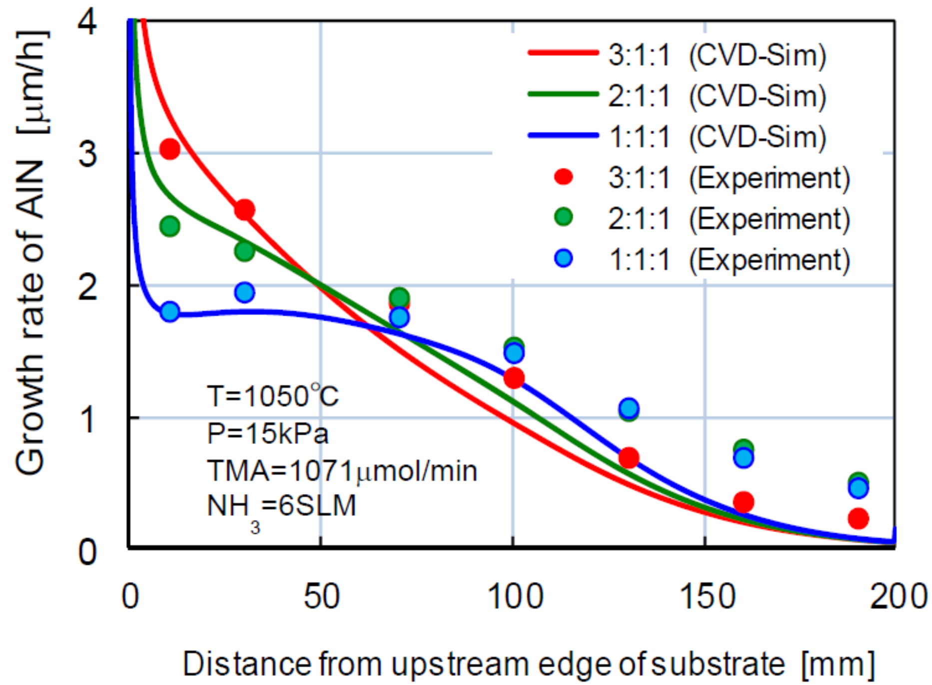


AlN growth in 6x8” Taiyo Nippon Sanso UR 26K reactor

Growth rate vs total flow



Growth rate as a function of the carrier



Modeling allows control of AlN growth rate value and growth rate uniformity over the 8” wafer

TAIYO NIPPON SANSO

Data: A. Ubukata et al., Phys. Status Solidi C 1-4 (2013)

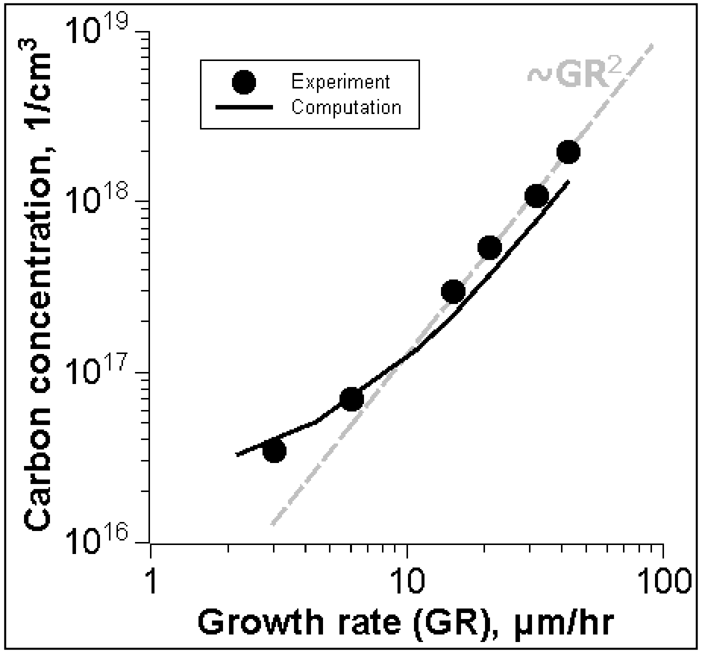
Carbon incorporation in GaN

Carbon is the impurity commonly used for fabrication of high-resistance GaN buffer layers in high power electronic devices. On the other hand, carbon in GaN is undesirable in some applications.

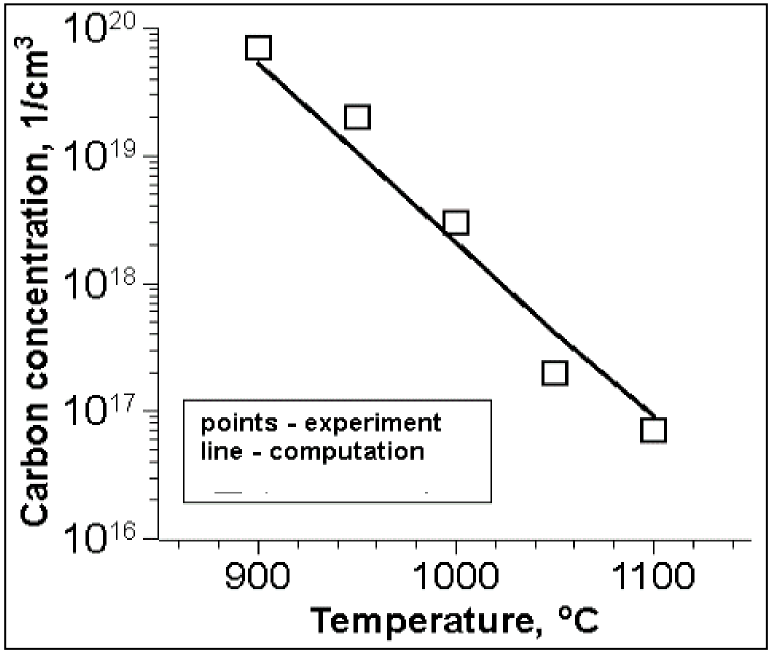
The rate of carbon incorporation depends on many factors and has to be controlled accurately.

Data: W. Lundin et al, ICMOVPE-2018

Effect of growth rate



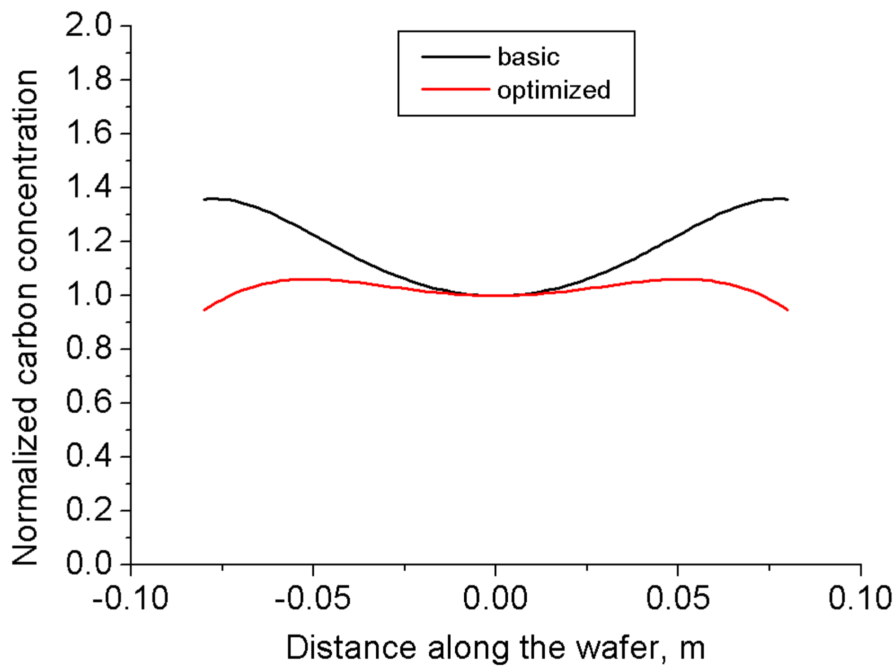
Effect of temperature



Optimization of Carbon in 8” GaN growth

Carbon concentration

- Carbon incorporation rate depends on many parameters
- It is very difficult to achieve good carbon uniformity for large-diameter wafers
- Advanced optimization of growth recipe is necessary

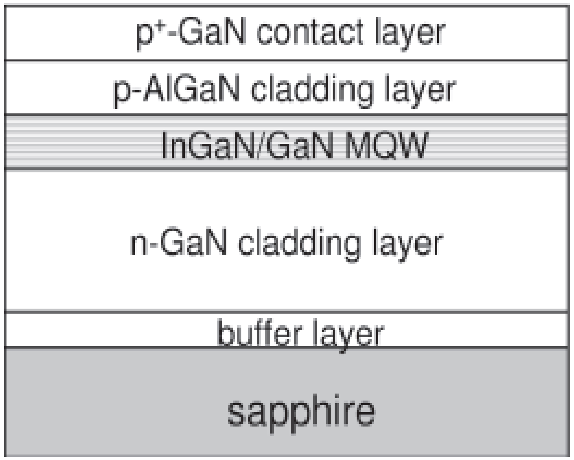


Simulations allows to find the growth conditions providing appropriate carbon concentration in the growing GaN layer and uniform carbon concentration over the surface of 8” wafer

Modeling of the characteristics of III-Nitride device heterostructures grown by MOCVD

STREEM-InGaN software

What is the best heterostructure design?



Device simulations can be used to answer the question

Modeling of LED operation

- ✓ Band diagrams
- ✓ Carrier concentrations
- ✓ Electric field
- ✓ R^{rad}, R_i^{nonrad}, IQE
- ✓ Emission spectra

N_{MQW}, X_{In}, δ_{QW}, N_A, ….

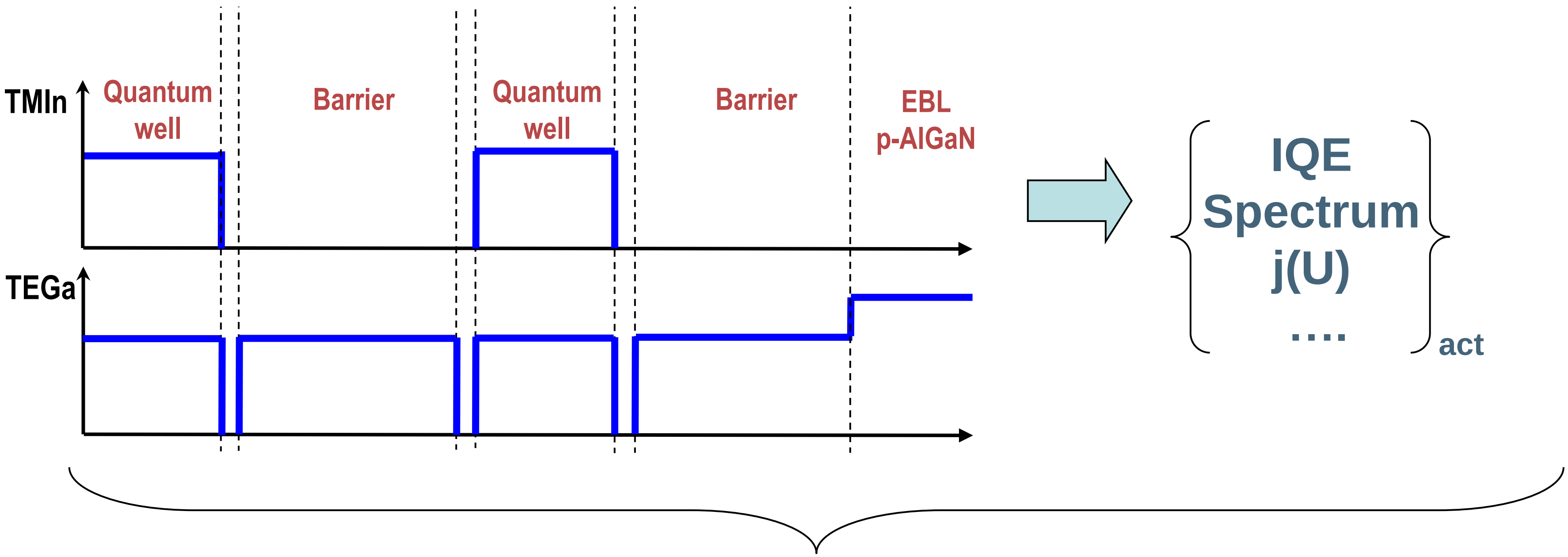
Over and over again to find the desirable structure design

$\{$ Number of QWs, Indium content, QW thickness, Doping level, ……. $\}_{des}$ → $\{$ IQE, Spectrum, j(U), …. $\}_{des}$

Desirable design → **Desirable characteristics**

Let's try to grow the heterostructure

Recipe for the structure growth



However, there is a difference between desirable and actual characteristics

What is the reason?

Main origins of the difference between desirable and actual heterostructures

- ✓ **Actual composition profile across the heterostructure**
- ✓ **Dislocation density**
- ✓ **Strain profile and relaxation degree in the structure**

Concept of simulations

Input

- Type of MOCVD reactor
- Recipe

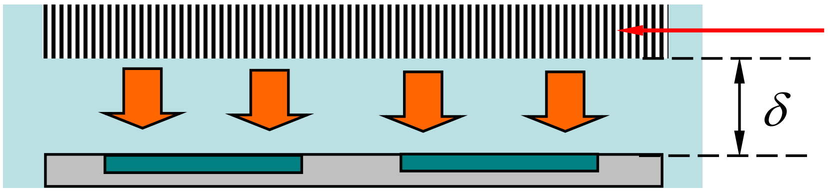
STREEM InGaN

- Model of growth and indium segregation
- Model of epitaxial stress relaxation
- Dislocation dynamics model
- Effect of strain on indium incorporation

Results

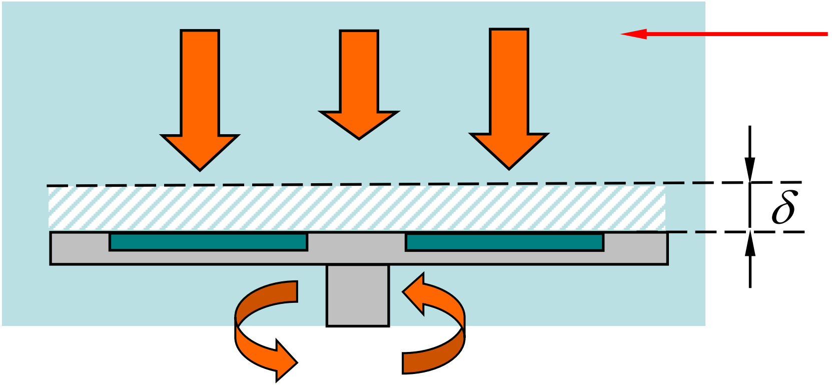
- Indium composition profile
- Strain distribution
- Dislocation density and distribution

Diffusion boundary layer in typical MOCVD reactors



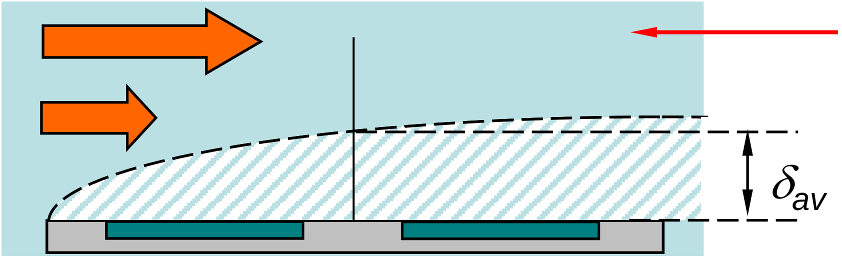
Close Coupled Showerhead

- Boundary layer has insufficient place to form, diffusion occurs through the fixed gap



Rotating Disk Reactor

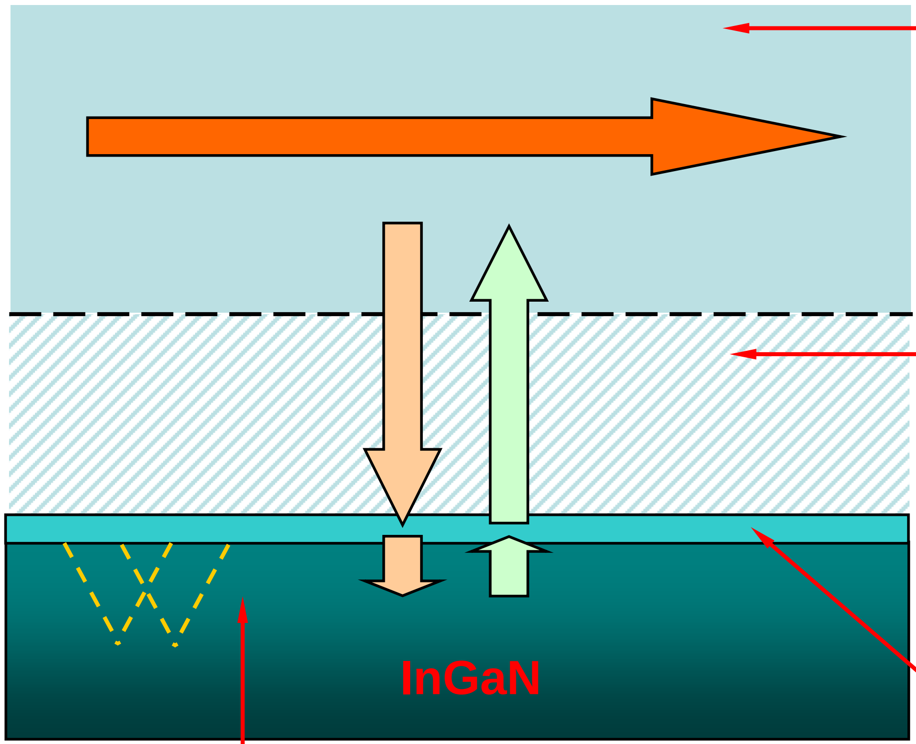
- Narrow rotation boundary layer is formed due to the dominant susceptor rotation



Horizontal/Planetary Reactor

- Non-uniform wall boundary layer is formed due to the dominant gas flow

Approach to unsteady modeling of InGaN/GaN MOCVD



Gas flow core

- Unsteady supply of precursors TMIn, TMGa, TEGa and NH_3 with carrier N_2 and H_2

Diffusion boundary layer

- Diffusion transport of gas species to/from the interface

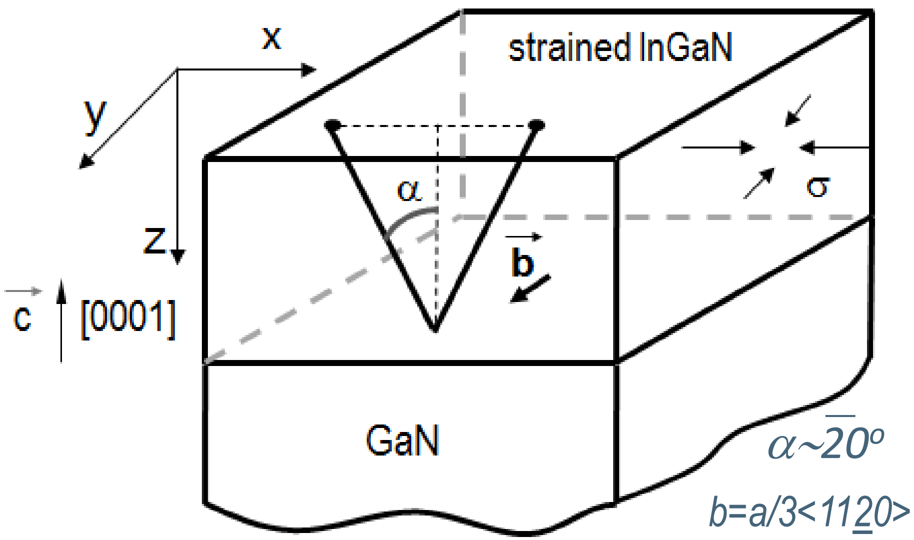
Adsorbed layer

- Unsteady balance of adsorbed atoms In, Ga, N, H
- Mass exchange with gas (adsorption/desorption)
- Mass exchange with crystal (incorporation/decomposition)

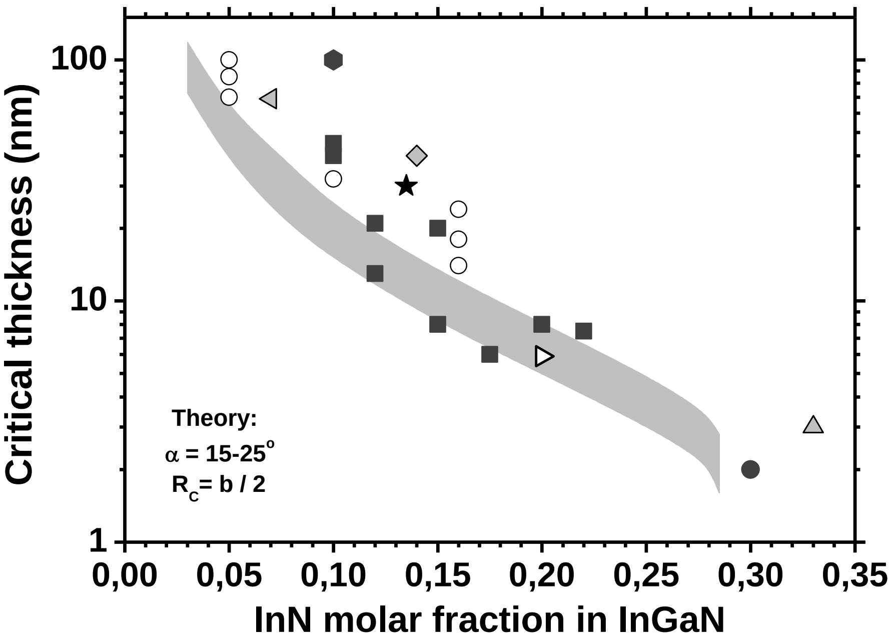
Crystal

- Unsteady formation of composition profile in InGaN/GaN
- Generation of dislocations

(0001) InGaN/GaN: critical layer thickness



V-shaped edge-type dislocation half-loop



V-shaped Dislocation half-loops:

- *are generated at the growth surface and frequently climb down to the InGaN/GaN interface*
- *are observed on both sapphire and bulk GaN substrates*
- *present in thick layers with low x_{In} and MQWs of various compositions*
- *density is order/orders of magnitude higher than the TD density in underlying GaN*

A.V. Lobanova et al., Appl. Phys. Lett. 103 (2013) 152106

European Union FP7 Project

Study of composition profile in LED structures

MOCVD

Microscopy

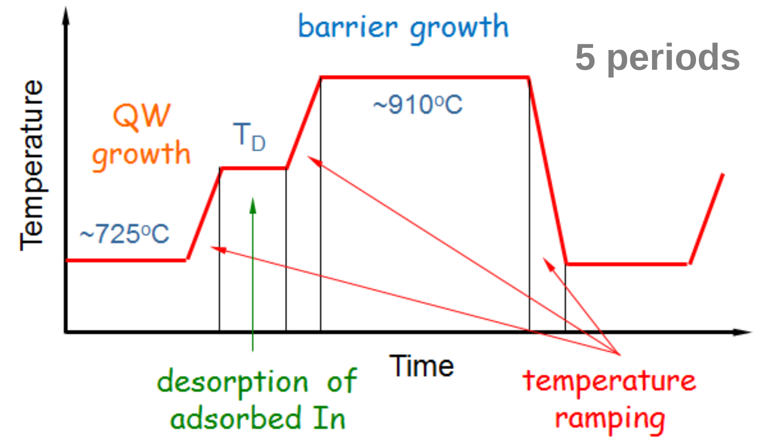
MQW structure with different temperatures after QW

Characterization:

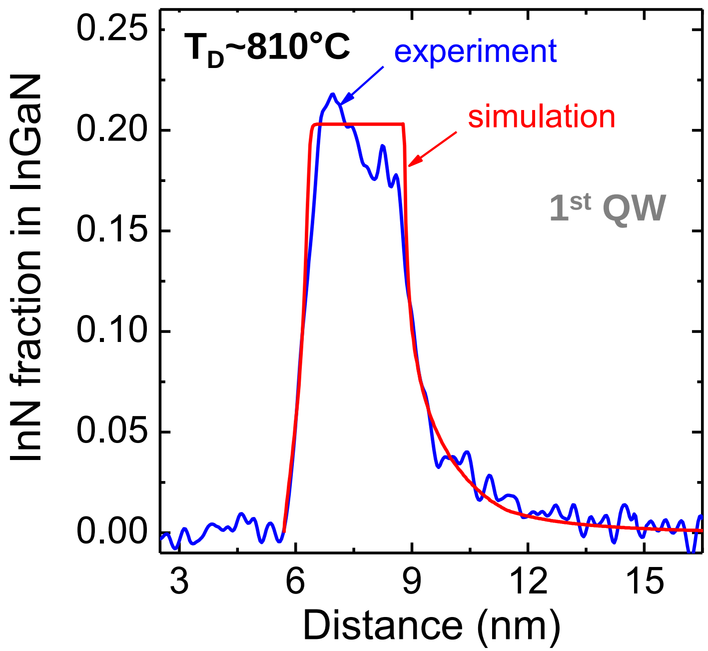
- Dark-Filed Electron Holography
- High Resolution TEM

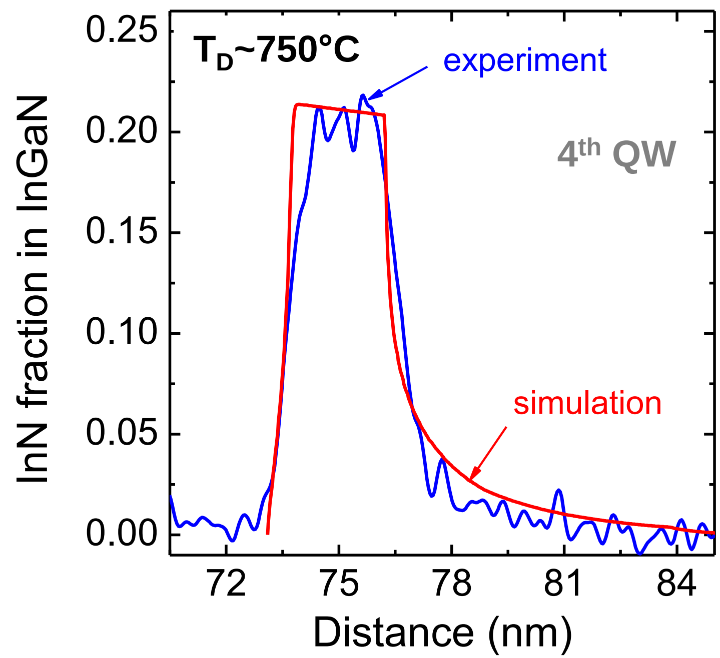
Simulation:

- STREEM InGaN



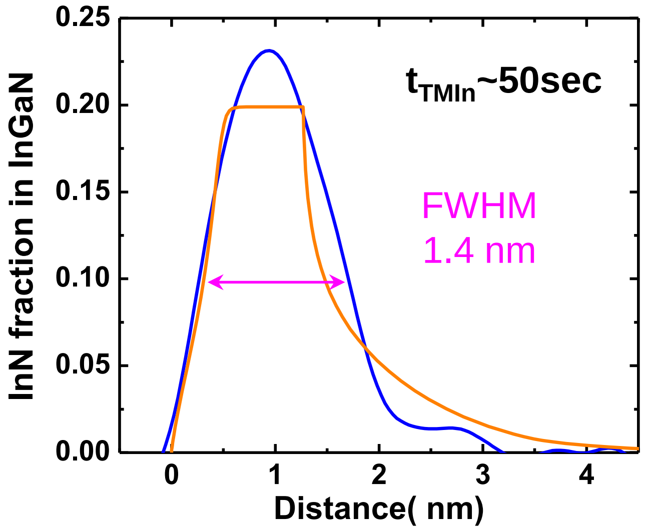
Indium profile vs barrier temperature

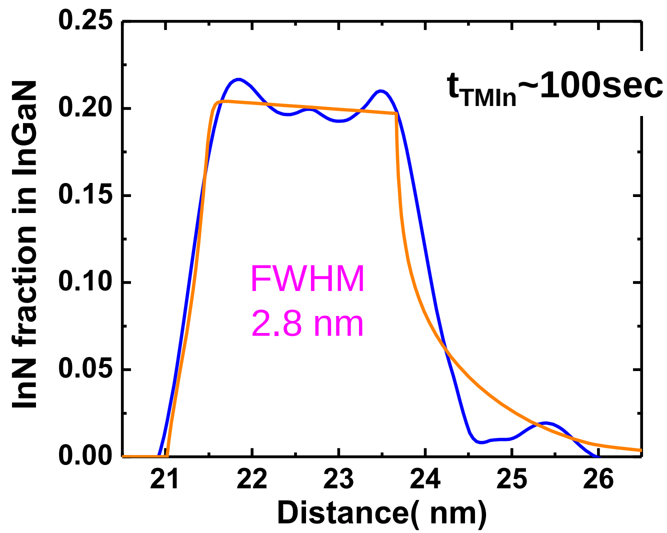




A. Segal et al., presented at IWN-2014, August 24-29, Wroclaw, Poland (2014)

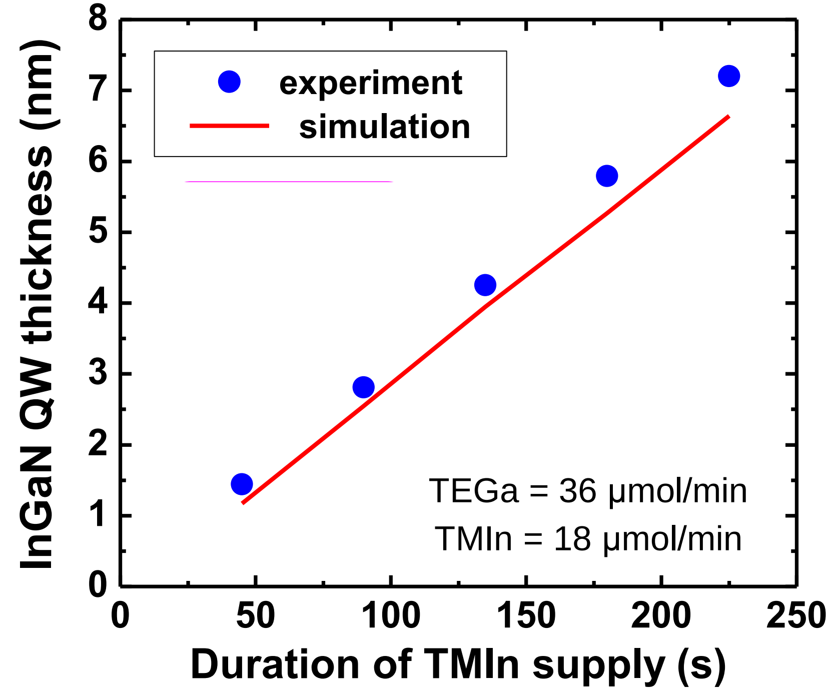
Effect of TMIn supply duration





simulation
from DFEH data

A. Segal et al., presented at IWN-2014, August 24-29, Wroclaw, Poland (2014)



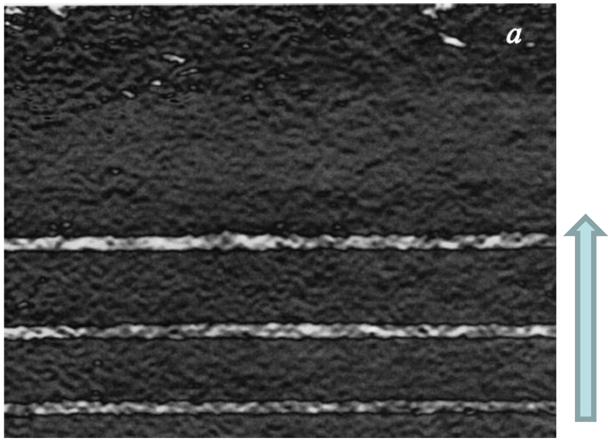
Strain relaxation in MQW LED structure

Ioffe Institute

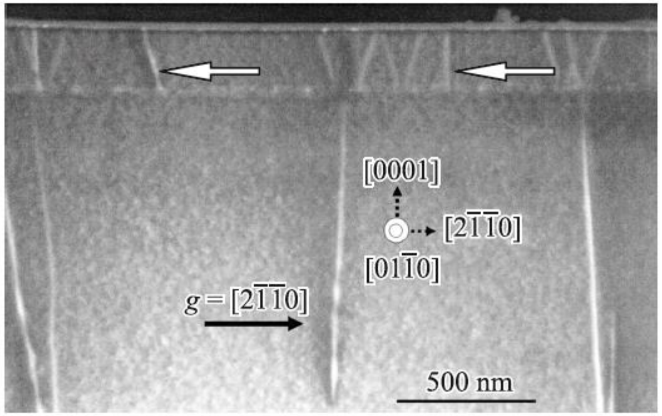
MQW structure with strain relaxation: experiment

MQW structure: Sakharov et al., Semiconductors, 43/6, 841 (2009)

- ✓ Structure with different number of QWs have been grown: one QW (G1) – three QWs (G3) – five QWs (G5)
- ✓ Indium content increases with the number of QWs
- ✓ Wavelength increases with the number of QWs
- ✓ Generation of additional dislocation half-loops in the active region



Distribution of deformations that confirms increase of the In content with the number of QWs

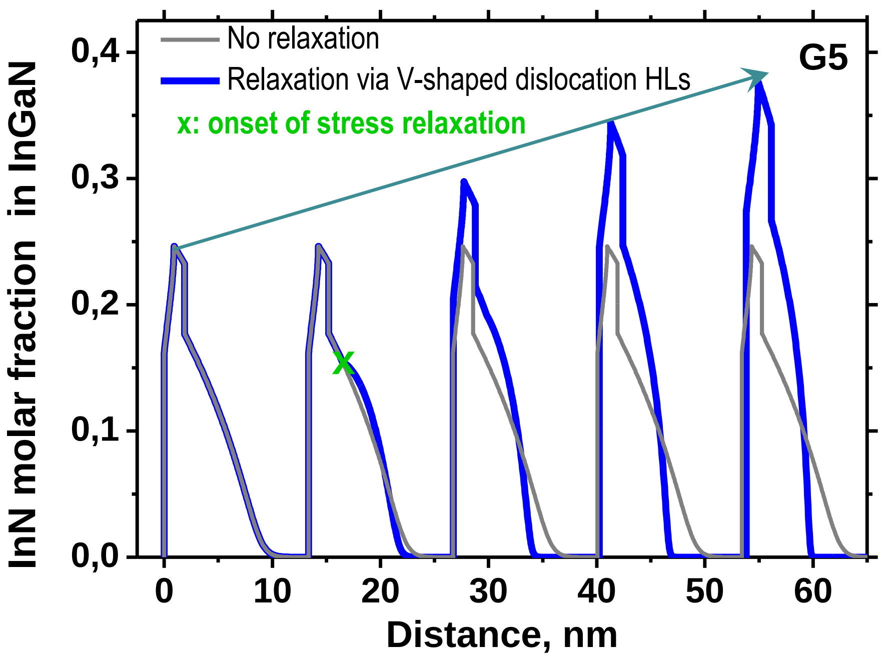


TEM image that confirms formation of new dislocations in the active region

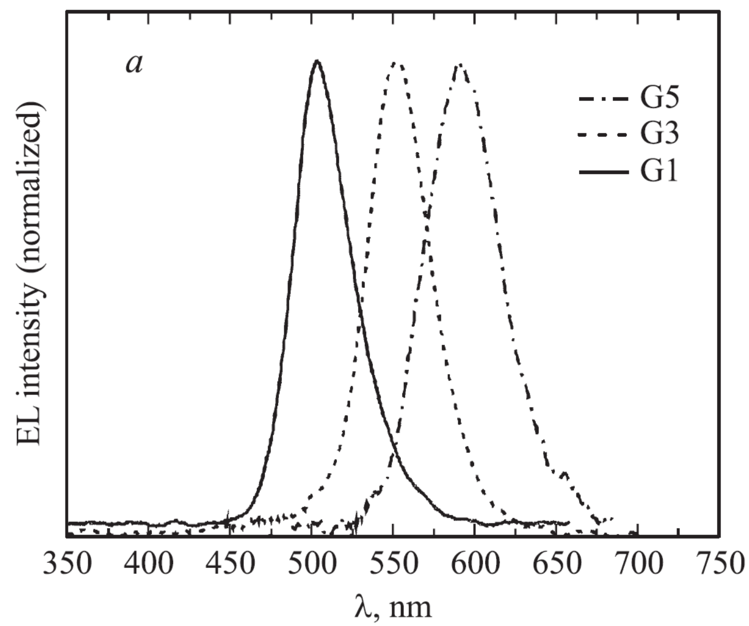
LED structure: composition and wavelength

- *wavelength/In content increases with the number of QWs: G1 - G3 - G5*
- *for the structure with 3 QWs, relaxation seems to occur in the 2nd /3rd QWs*

Composition profile: STREEM simulation



Shift of the EL wavelength with the number of QWs



Increase in the indium content due to partial stress relaxation agrees with the corresponding increase of the measured wavelength for the structures G1, G3, and G5

A.V. Lobanova et al., presented at ICNS-10, August 25-30, Washington, USA (2013)

Stress and dislocation behavior and wafer bowing in GaN growth on Silicon

STREEM-AlGaN software

Modeling approach

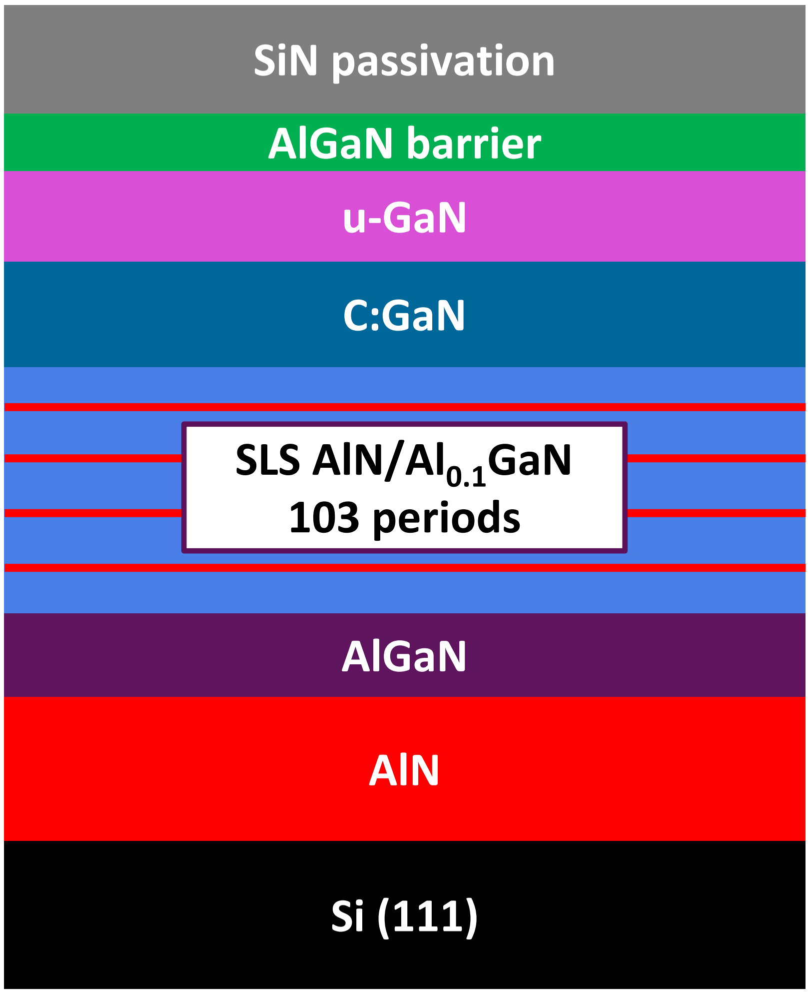
Input parameters:

- Type of the reactor
- Thickness and diameter od the substrate
- Properties of each layer in the stack: composition, doping, thickness
- Growth conditions

STREEM predictions:

- Curvature evolution of curvature at the stages of heating, growth, and cooling
- Stress relaxation and dislocation dynamics
- Crack formation during the growth and after cooling of the structure
- Influence of the process parameters on the through-wafer temperature drop and its contribution to the structure bow
- Stress state in the particular layers via processing of in-situ curvature data

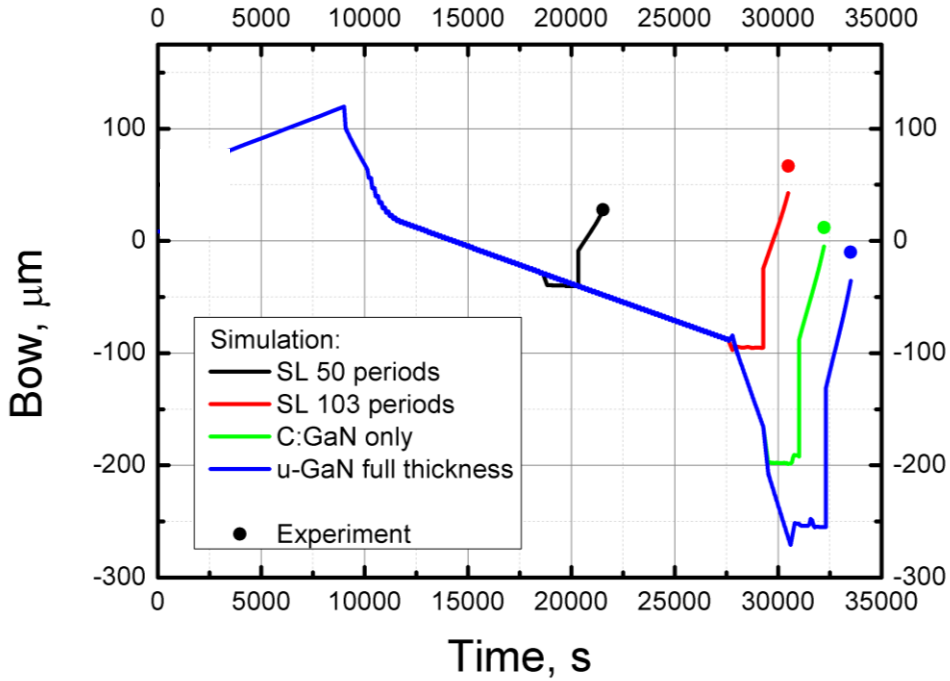
GaN-on-Si based HEMT epi-wafers with AlN/AlGaN superlattice buffer, grown in production-scale reactor

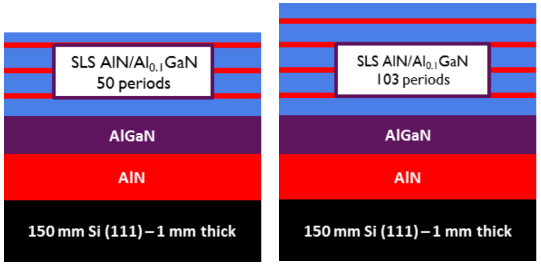


- ✓ GaN-on-Si based HEMT epi-wafers, grown in production-scale reactor
- ✓ AlN/AlGaN superlattice buffer

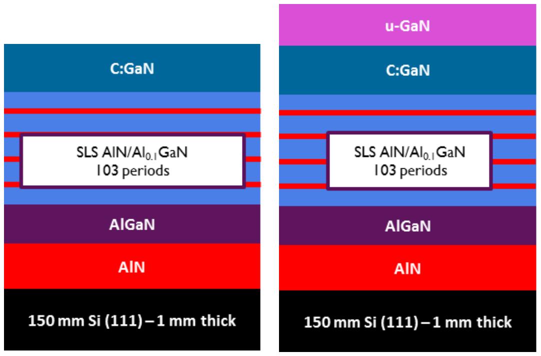
Japanese Journal of Applied Physics 58, SCCD26 (2019)

Stop-growth experiments





SL 50 periods   SL 103 periods

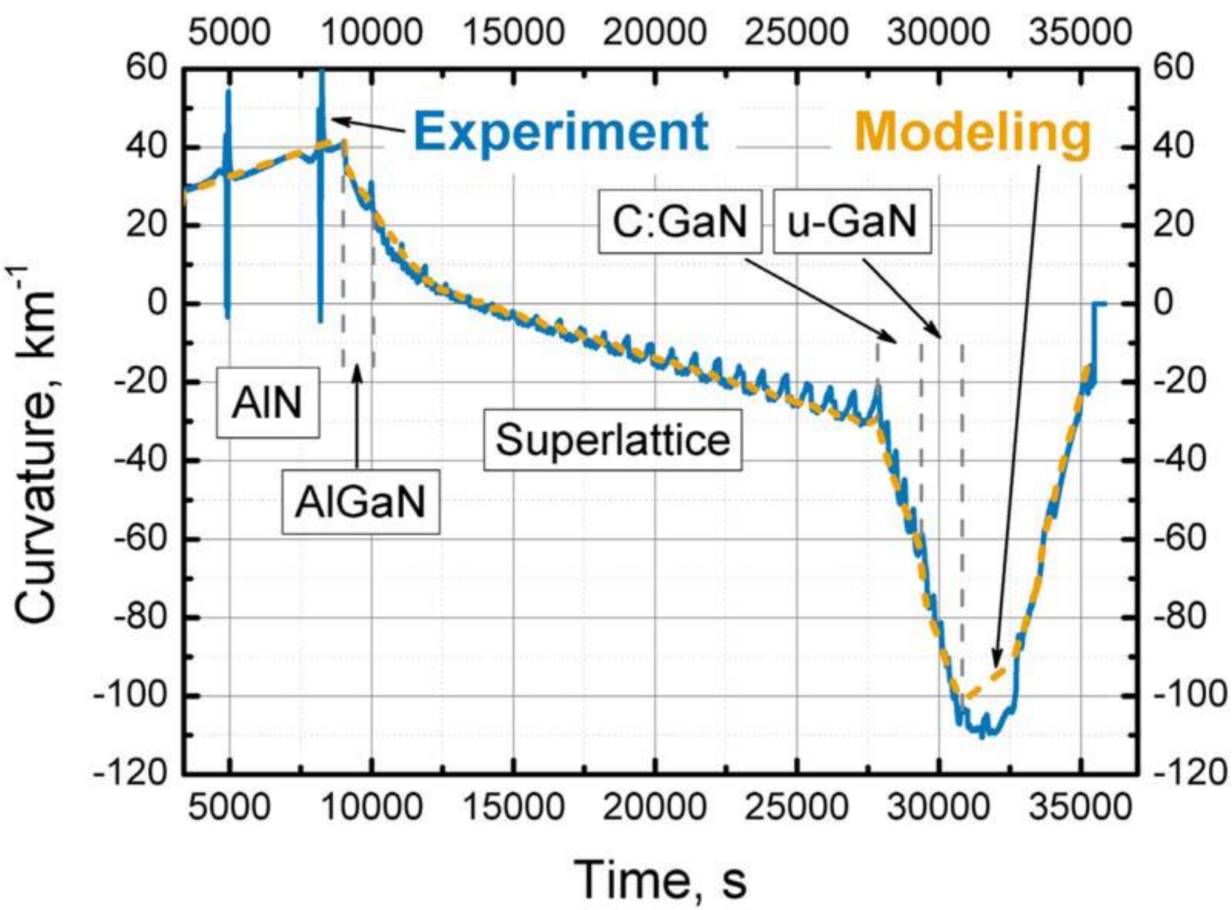


C:GaN only   u-GaN full thickness

Modeling reproduces stop-growth experiments designed to evaluate the effect of individual buffer parts on RT bow:

- RT bow is predicted for various thickness and composition of the stack
- Plastic relaxation in silicon wafer is not expected

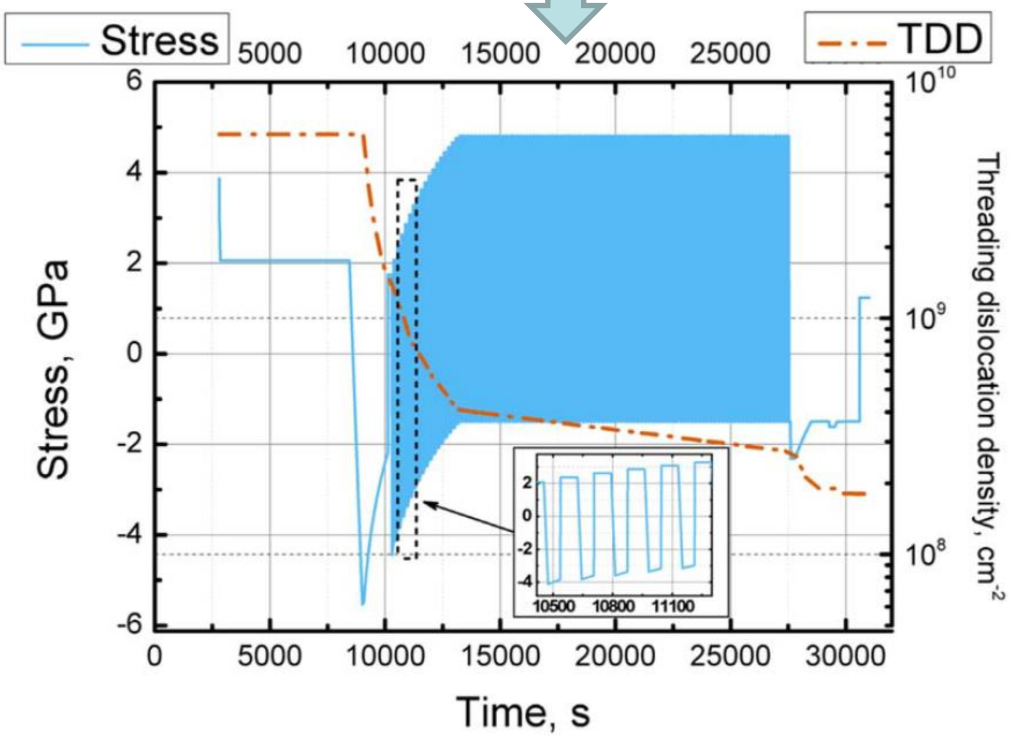
Curvature evolution



- Adjustment of the recipe provides almost zero curvature after cooling
- Linear variation of the curvature for the most part of the SL: weakly changing averaged stress

Analysis of the stress and TDD evolution in the SL

Computed temporal variation of the stress and dislocation density (the inset shows the details of the stress evolution in the bottom part of the SL)



- ✓ AlGaN/AlN superlattice is effective in filtering the dislocations, whose density keeps reducing in the C:GaN and u-GaN layers grown on top of the SL with no nucleation of new dislocations
- ✓ Unintentional gallium incorporation into nominal AlN layers in the SL has been identified as a factor governing bow and stress evolution
- ✓ Proper design of the epitaxial structure and optimization of the process parameters provides final reduction of TDD down to about $2 \cdot 10^8$ cm^{-2} with the good structural uniformity over 6" wafers and a residual bow below 50 µm

Growth of GaN by HVPE

Hydride Epitaxial GaN Simulator (HEpiGaNS) or VR HVPE

Modeling approach

Input parameters:

- Reactor geometry drawn by the user or imported from CAD file
- Operating temperature and pressure
- HCl and NH_3 flow rates

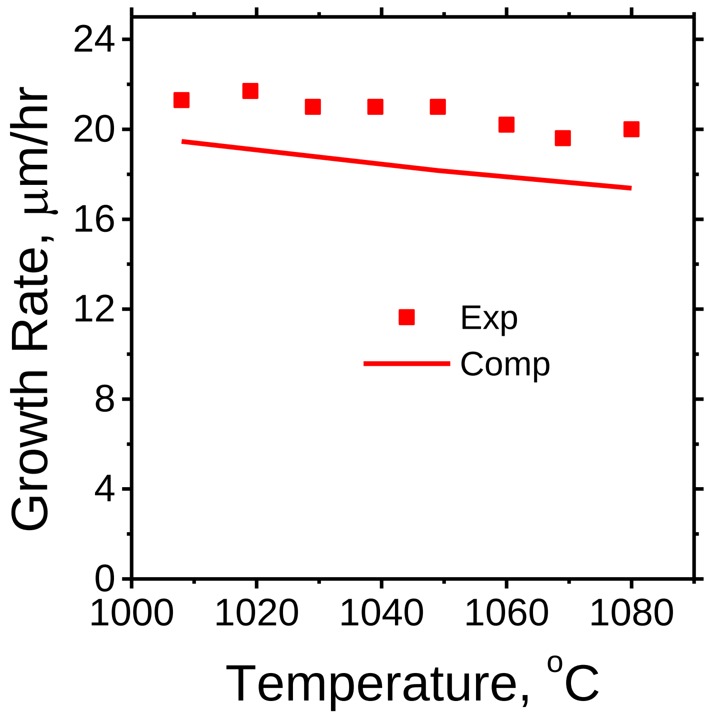
MOCVD process optimization:

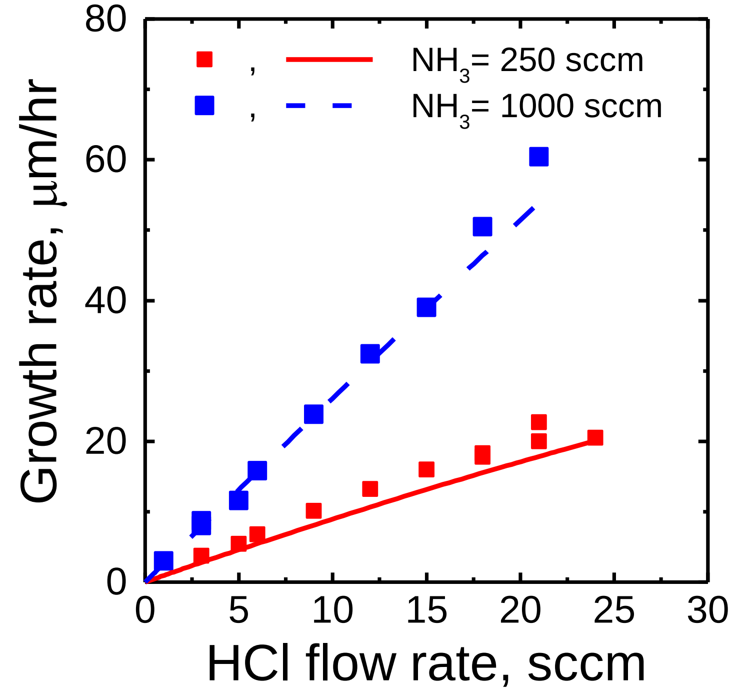
- Arrangement of gas species supply into the reactor providing
  - High GaN growth rate
  - Uniform GaN growth rate distribution over the substrate surface
- Increase of the efficiency of the source with liquid Ga
- Suppression of poly-GaN deposition on the reactor side walls

Dependence of GaN growth rate on growth conditions

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

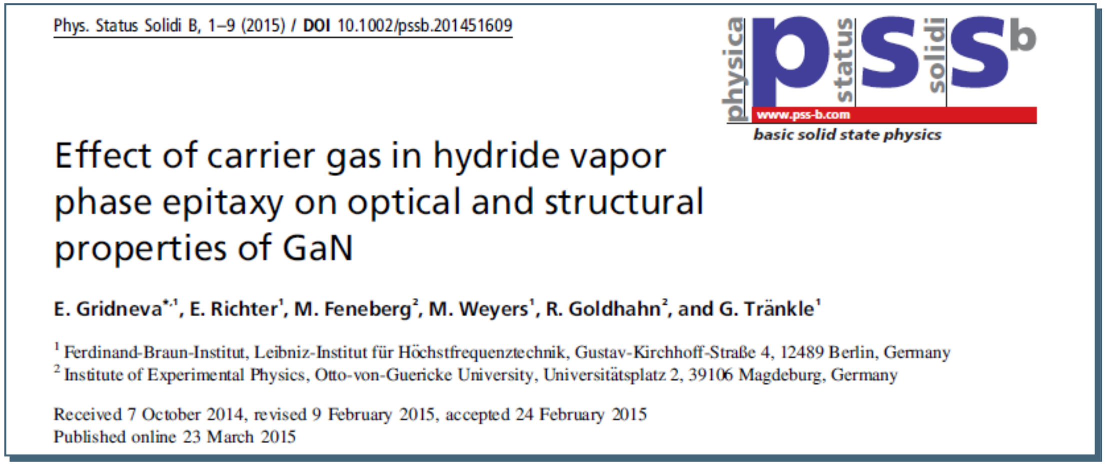
J. of Crystal Growth 270 (2004) 384





Computed and experimental dependencies of the GaN growth rate on temperature and HCl flow rate are in good quantitative agreement

Optimization of GaN growth by HVPE in AIXTRON Vertical HVPE Reactor


Phys. Status Solidi B, 1–9 (2015) / DOI 10.1002/pssb.201451609

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Effect of carrier gas in hydride vapor phase epitaxy on optical and structural properties of GaN

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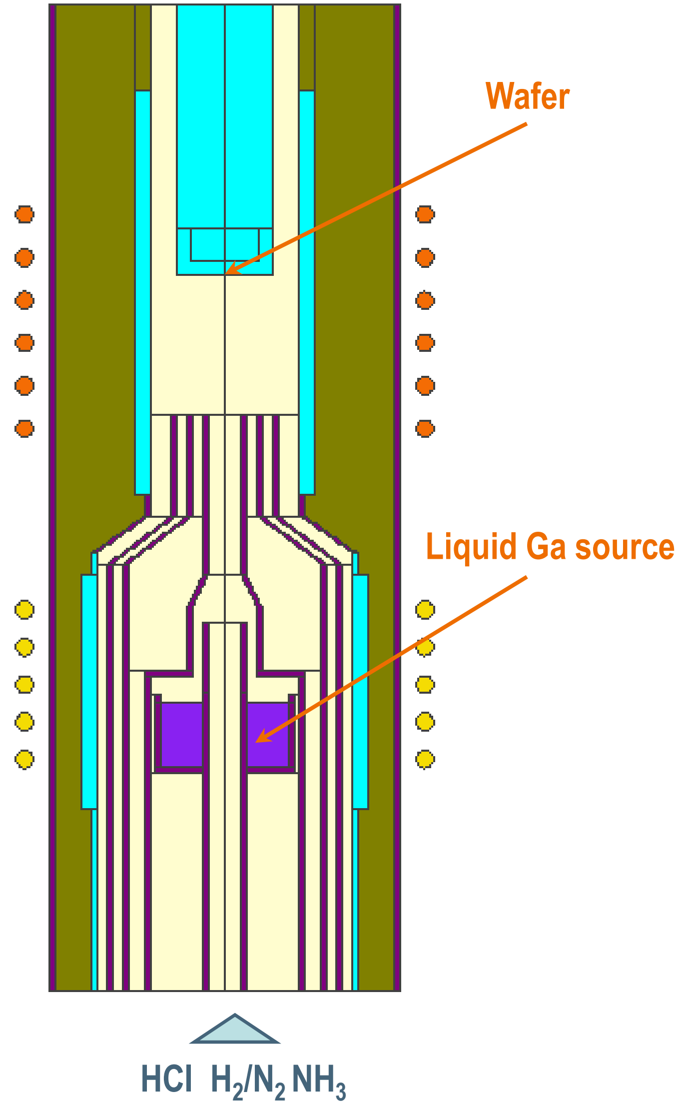

Using a combination of experiments and modeling 3 mm thick 3” GaN crystal was grown without cracking

Thank you for your attention!