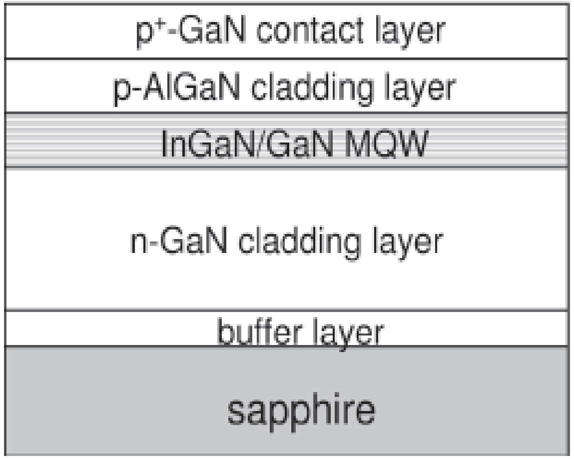
STREEM: STRain Engineering in Electronic Materials

InGaN Edition

2014

STR Group

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, ….

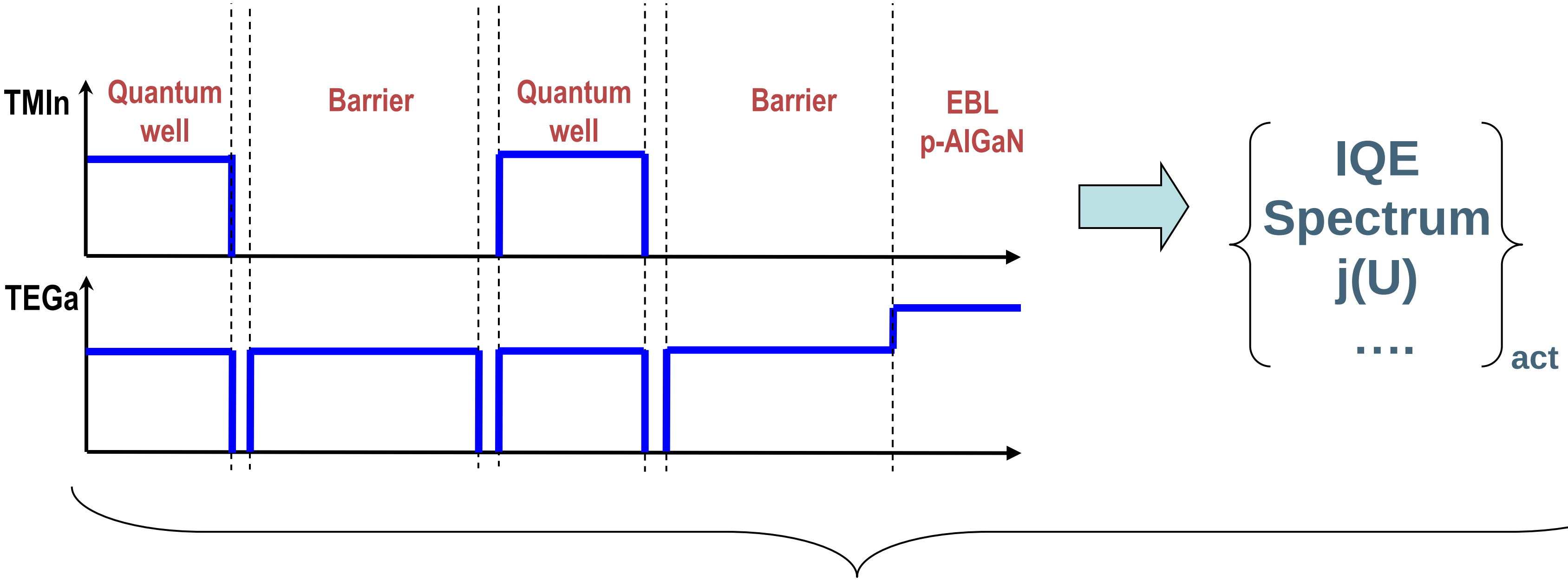
Over and over again to find the desirable structure design

$$\left\{ \begin{array}{c} \text{Number of QWs} \\ \text{Indium content} \\ \text{QW thickness} \\ \text{Doping level} \\ \ldots\ldots. \end{array} \right\}_{des} \Rightarrow \left\{ \begin{array}{c} \text{IQE} \\ \text{Spectrum} \\ j(U) \\ \ldots. \end{array} \right\}_{des}$$

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

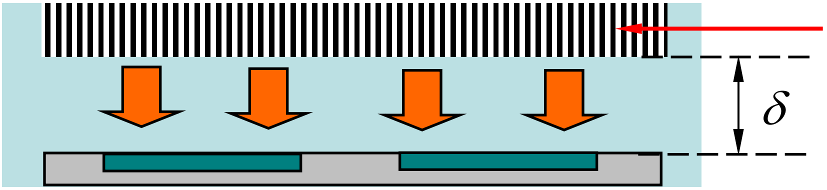
STREEM InGaN

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

Results

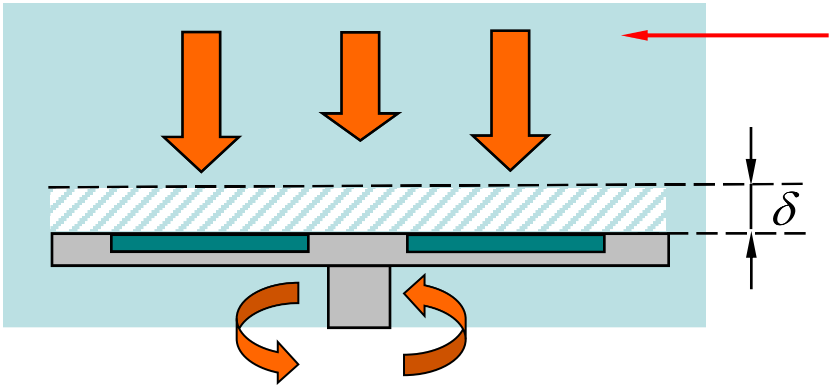
- Indium composition profile
- Strain distribution
- Dislocation density and distribution

Diffusion boundary layer in typical MOCVD reactors



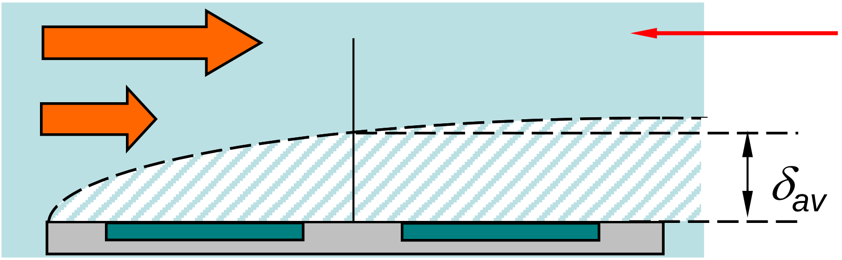
Close Coupled Showerhead

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



Rotating Disk Reactor

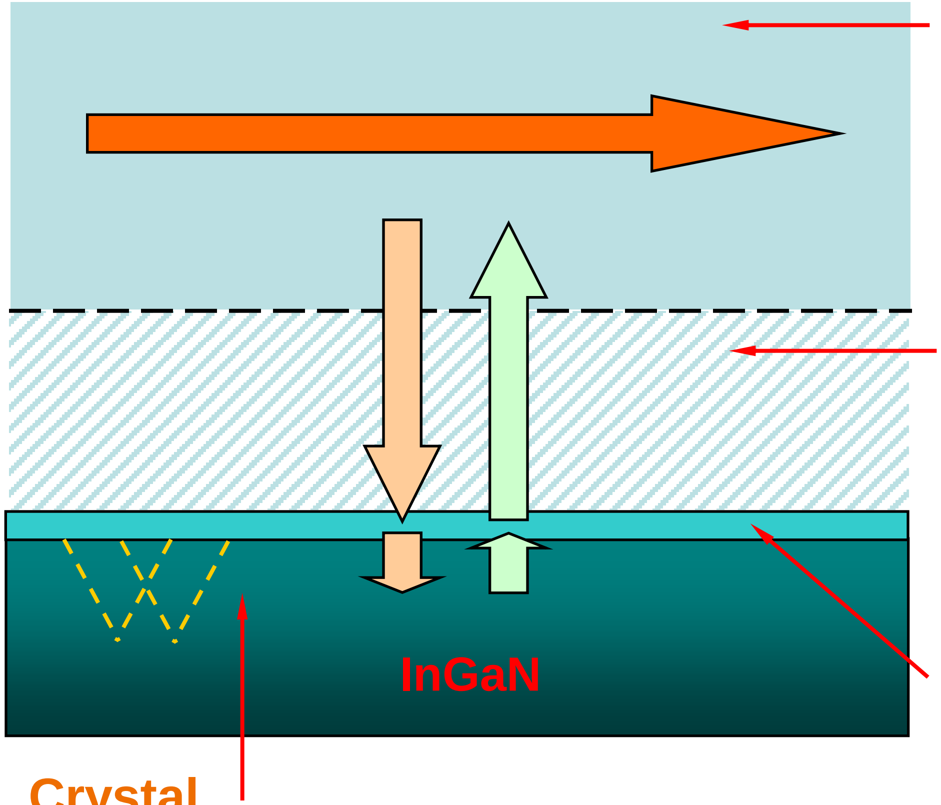
- Narrow rotation boundary layer is formed due to the dominant susceptor rotation



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

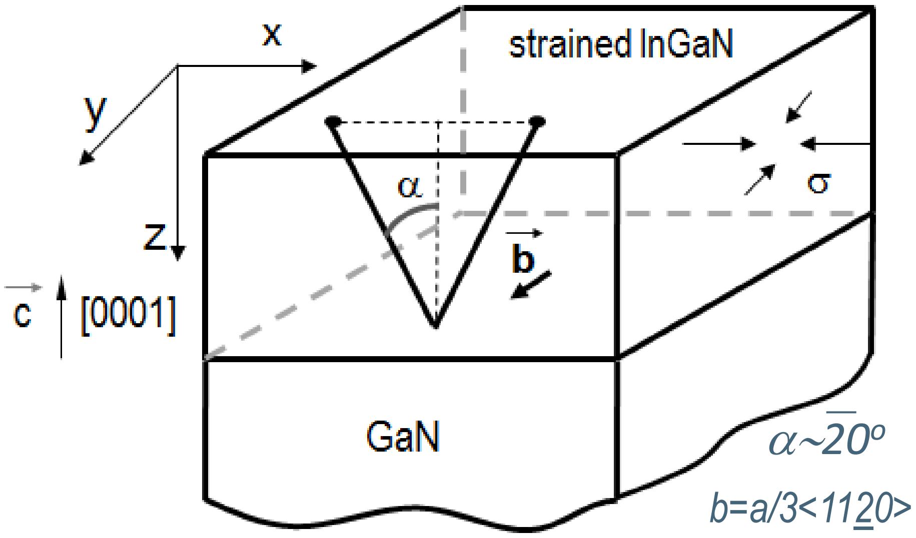
Adsorbed layer

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

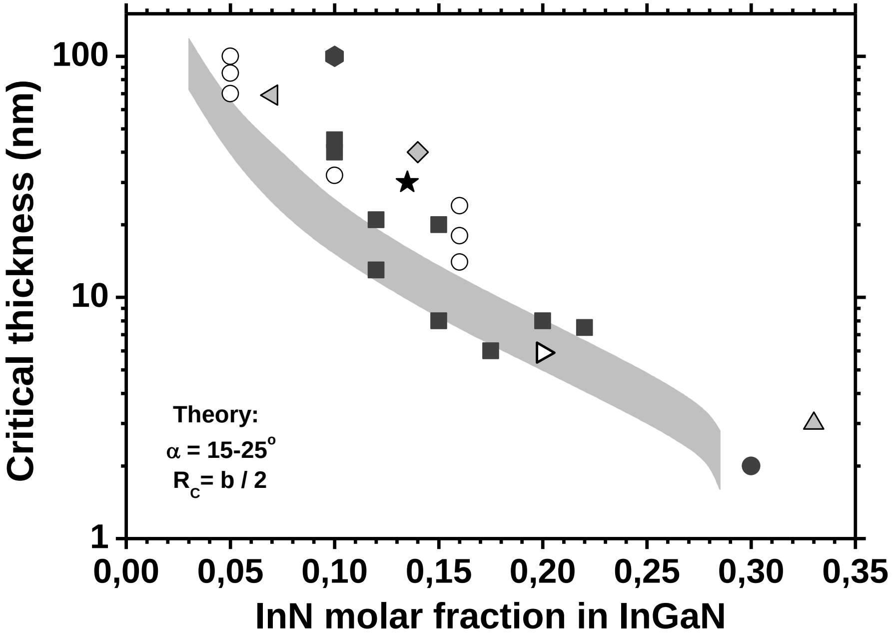
Crystal

- 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

NEWLED

European Union FP7 Project

Study of composition profile in LED structures

OSRAM
Opto Semiconductors

MOCVD

CEMES
TOULOUSE

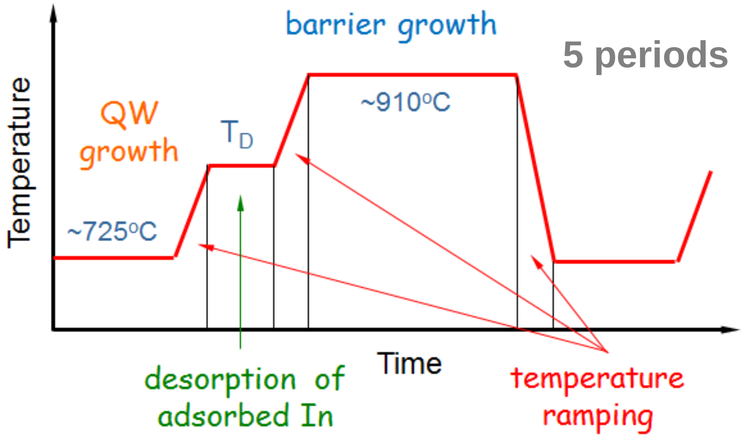
cnrs
dépasser les frontières

Microscopy

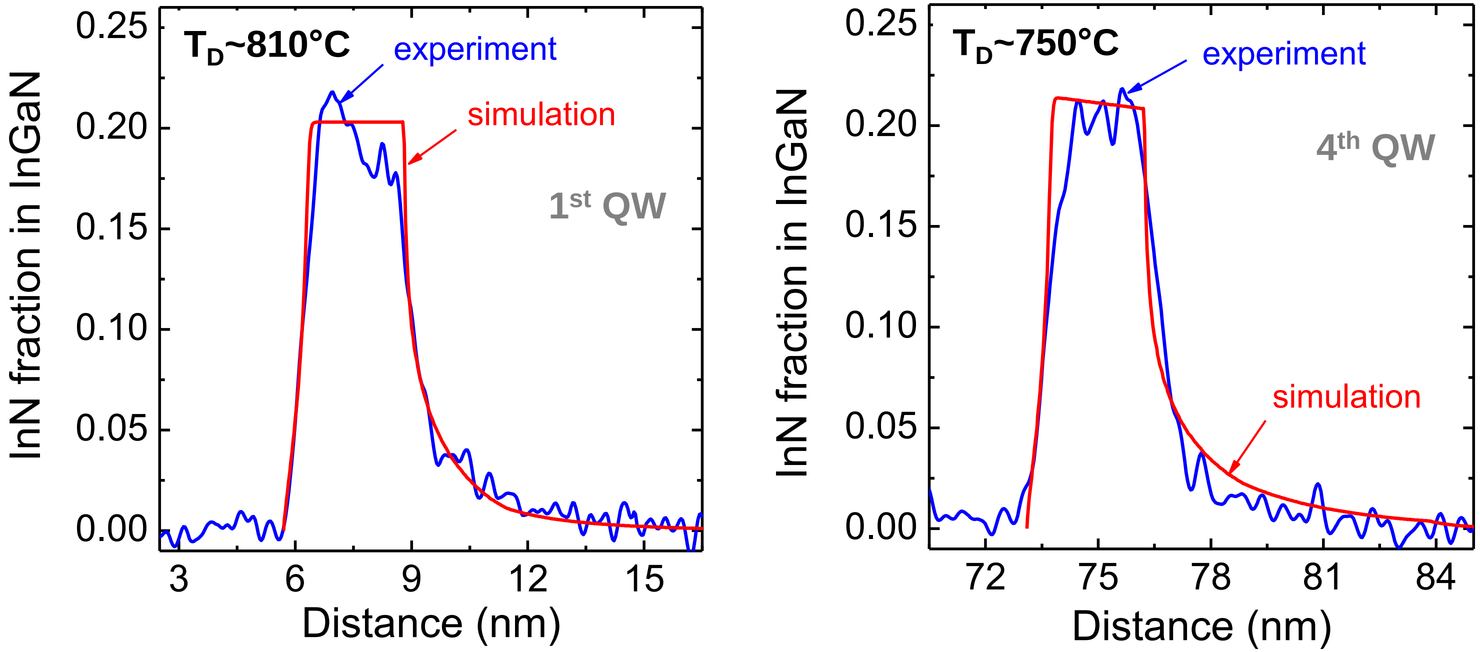
MQW structure with different temperatures after QW

Characterization:
- Dark-Filed Electron Holography
- High Resolution TEM

Simulation:
- **STREEM InGaN**

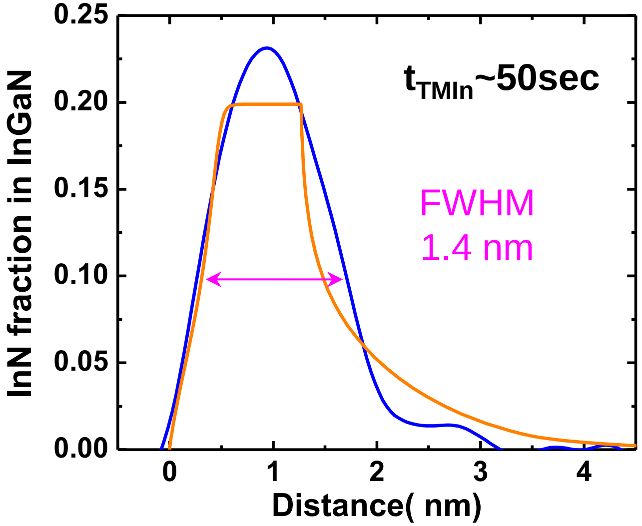


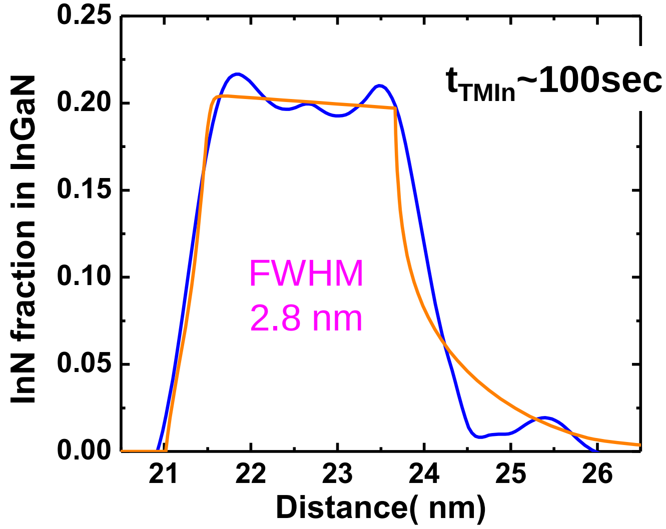
Indium profile vs barrier temperature



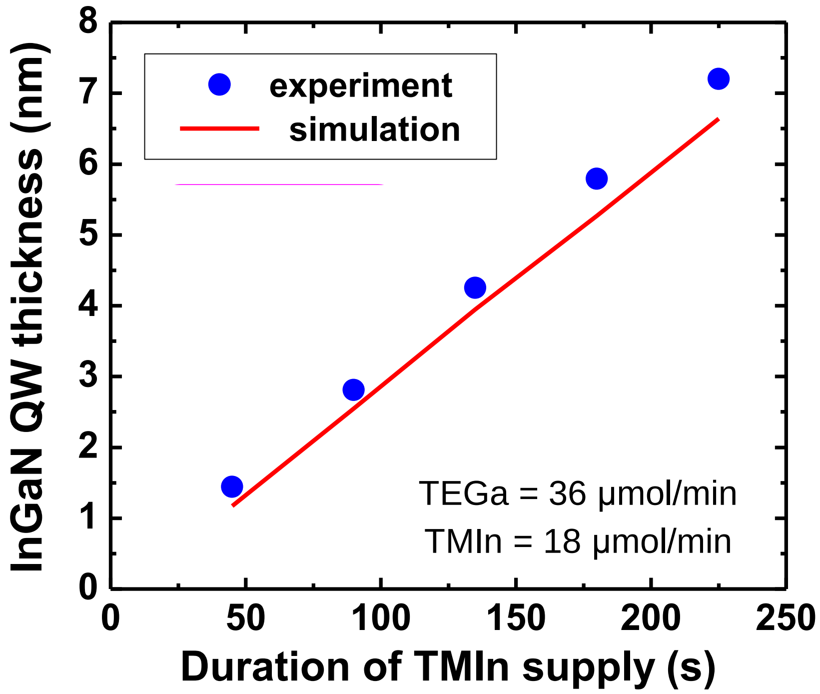
A. Segal et al., presented at IWN-2014, August 24-29, Wroclaw, Poland (2014)

Effect of TMIn supply duration





— simulation
— from DFEH data



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

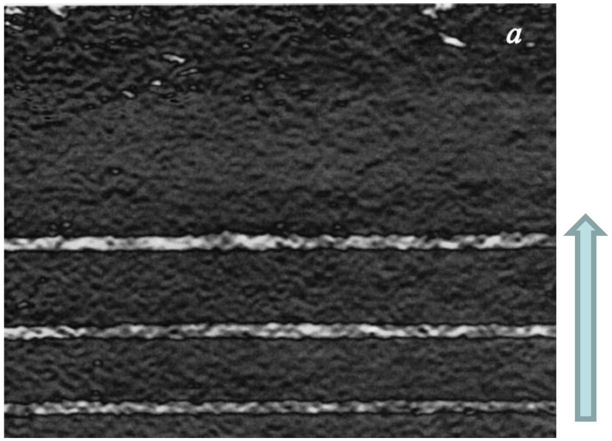
Strain relaxation in MQW LED structure

Ioffe Institute

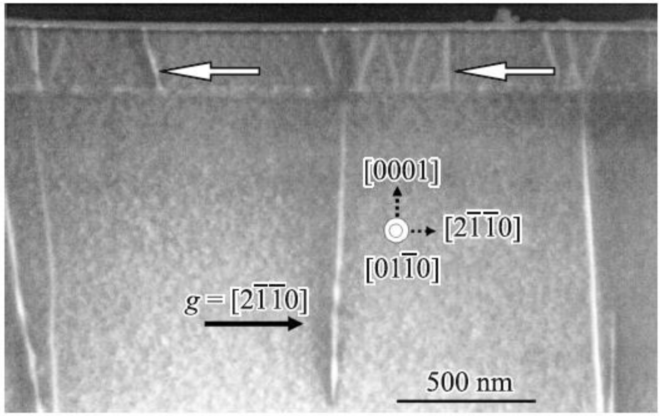
MQW structure with strain relaxation: experiment

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

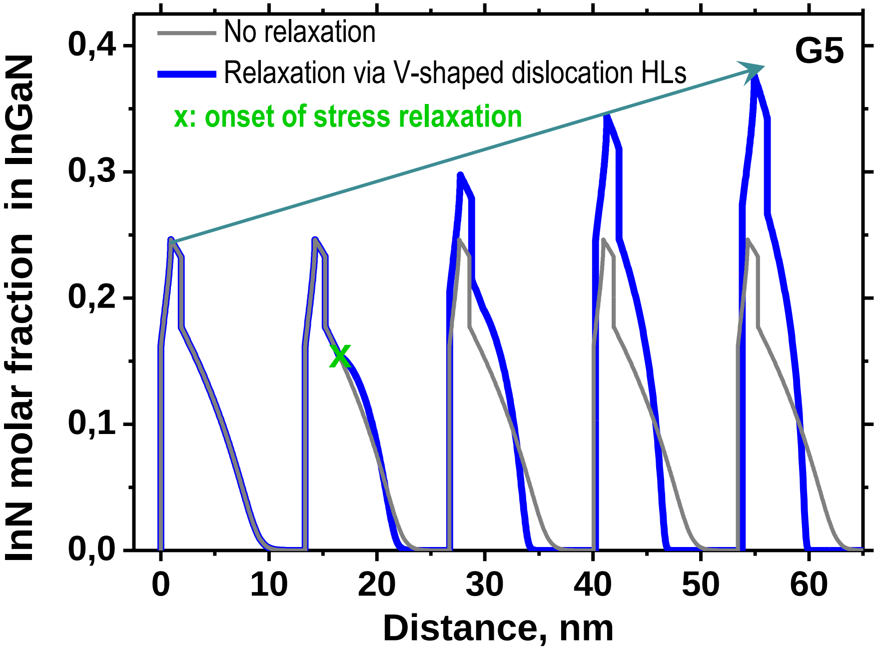


TEM image that confirms formation of new dislocations in the active region

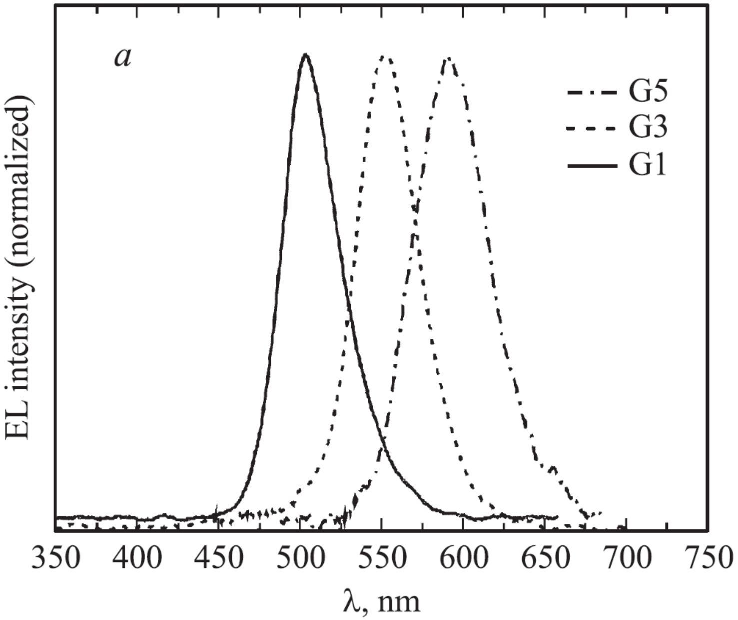
LED structure: composition and wavelength

- *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



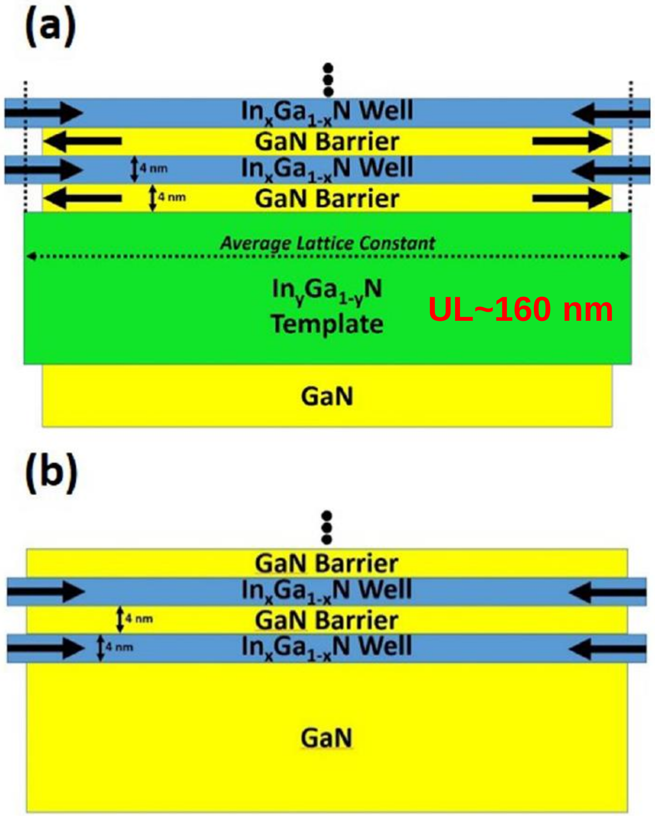
Increase in the indium content due to partial stress relaxation agrees with the corresponding increase of the measured wavelength for the structures G1, G3, and G5

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

Strain-balanced InGaN/GaN MQW

NC STATE UNIVERSITY

Strain balanced MQW structure



$$(a_{UL} - a_{barrier})h_{barrier} = (a_{QW} - a_{UL})h_{QW}$$

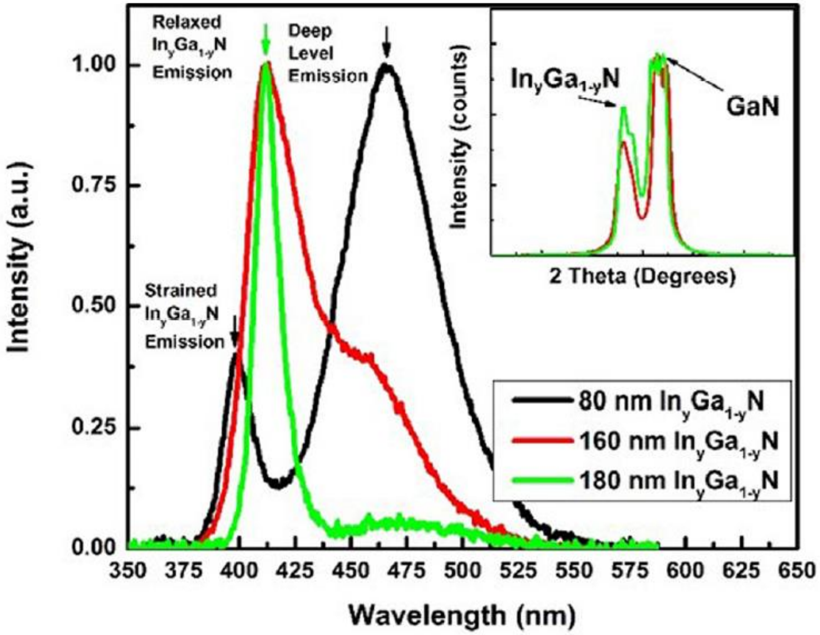
$$h_{barrier} = h_{QW} \Rightarrow x = 2y$$

- ✓ $In_xGa_{1-x}N$ MQW structure was grown directly on GaN buffer or with the use of $In_yGa_{1-y}N$ underlayers (ULs)
- ✓ Strain balance by adjusting the QW/barrier width and UL/QW composition
- ✓ Structures with x=0.16/y=0.08 and x=0.22/y=0.11
- ✓ Thick UL to provide its relaxation

D.M. Van Den Broeck et al., Appl. Phys. Lett. 105 (2014) 031107

Underlayer relaxation

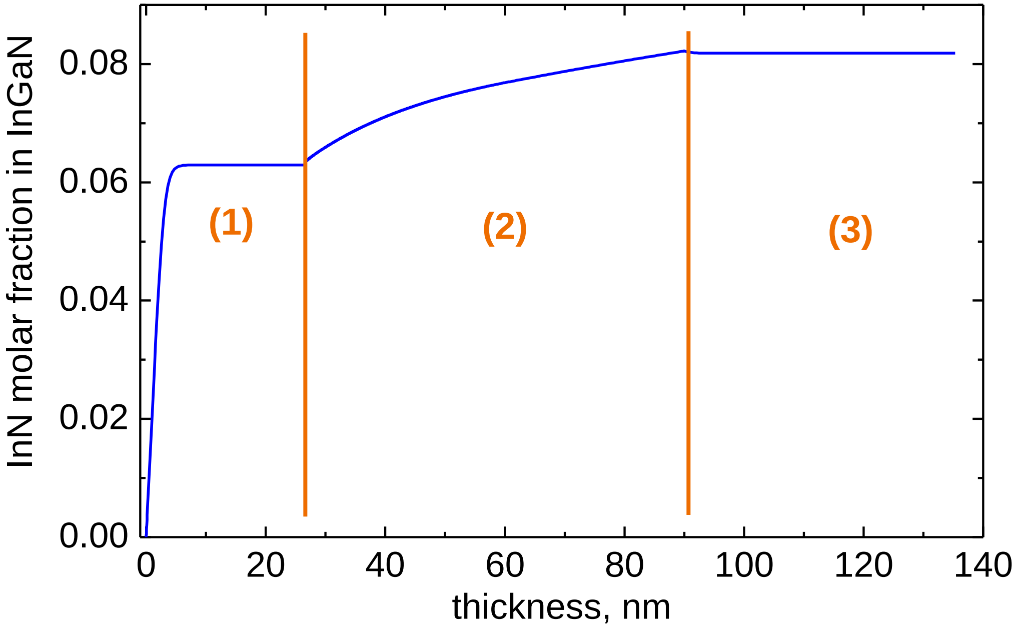
relaxation of InGaN UL: experiment



80 nm thick UL: still partly stressed

160nm/180 nm thick ULs: fully relaxed

relaxation of InGaN UL: STREEM modeling



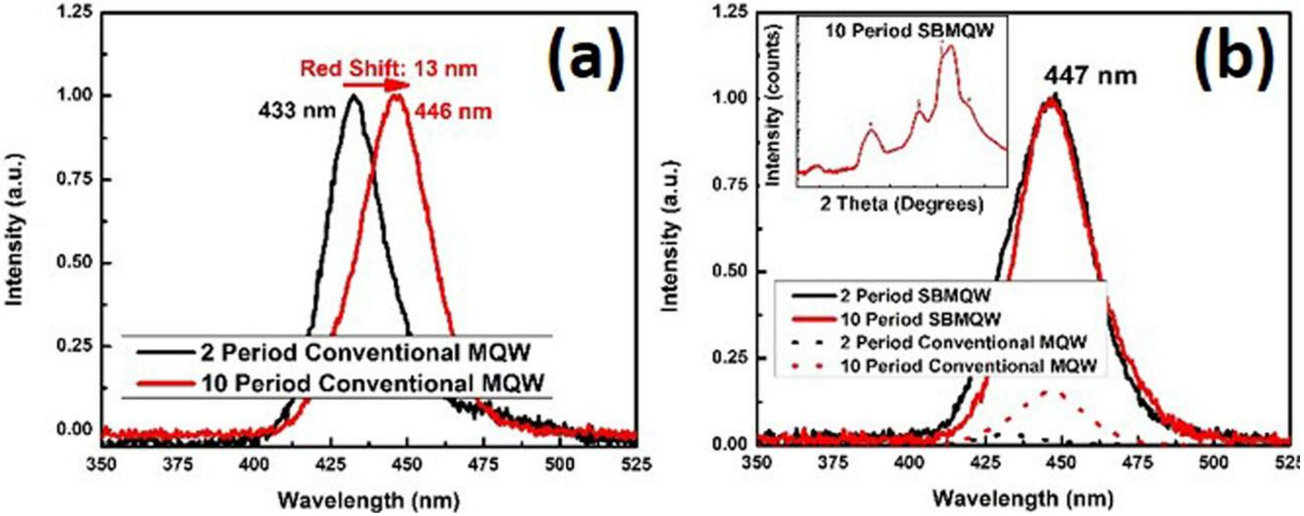
(1): no stress relaxation, X_{In}~const; CLT~30 nm
(2): stress relaxation, X_{In}~varied
(3): relaxed layer, X_{In}~const

160 nm thick InGaN underlayer (y=0.08) is fully relaxed

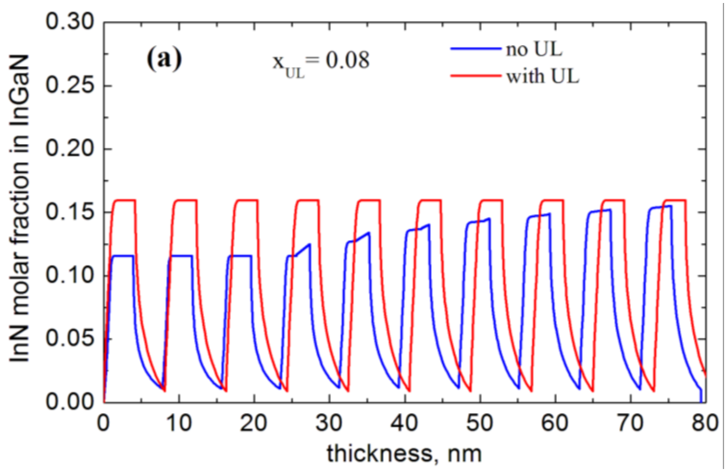
D.M. Van Den Broeck et al., Appl. Phys. Lett. 105 (2014) 031107

MQW composition and relaxation

experiment



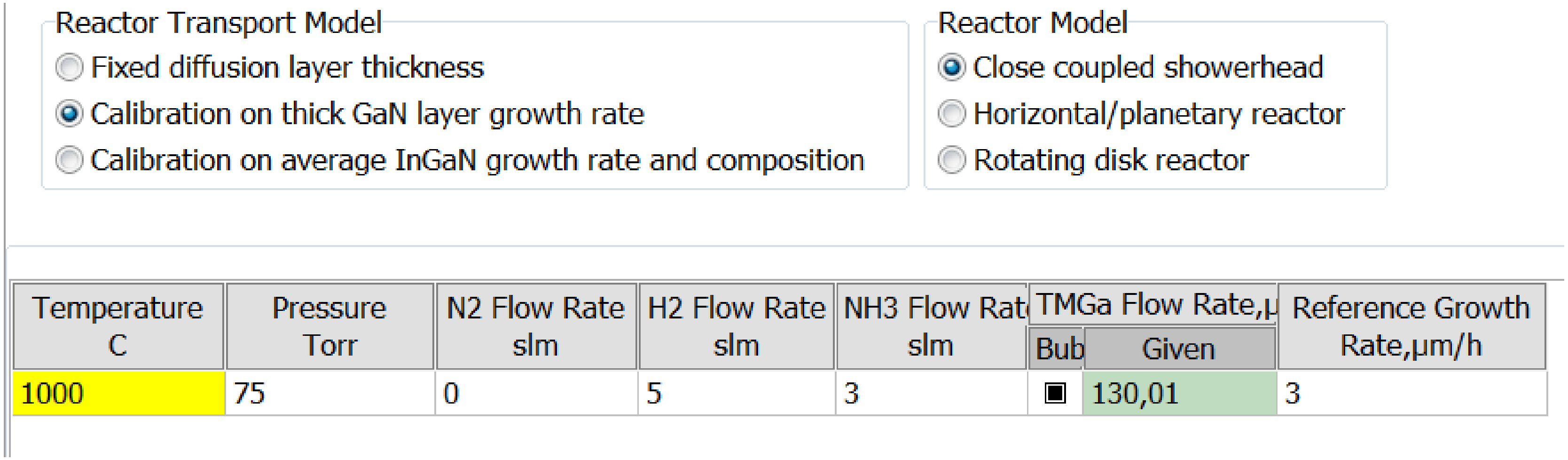
STREEM modeling



- Increased indium incorporation in 10 period conventional MQW due to relaxation
- Uniform indium composition and no relaxation for strain-balanced MQW (SBMQW)

D.M. Van Den Broeck et al., Appl. Phys. Lett. 105 (2014) 031107

STREEM-InGaN operation: transport model



Reactor Transport Model
- ○ Fixed diffusion layer thickness
- ● Calibration on thick GaN layer growth rate
- ○ Calibration on average InGaN growth rate and composition

Reactor Model
- ● Close coupled showerhead
- ○ Horizontal/planetary reactor
- ○ Rotating disk reactor

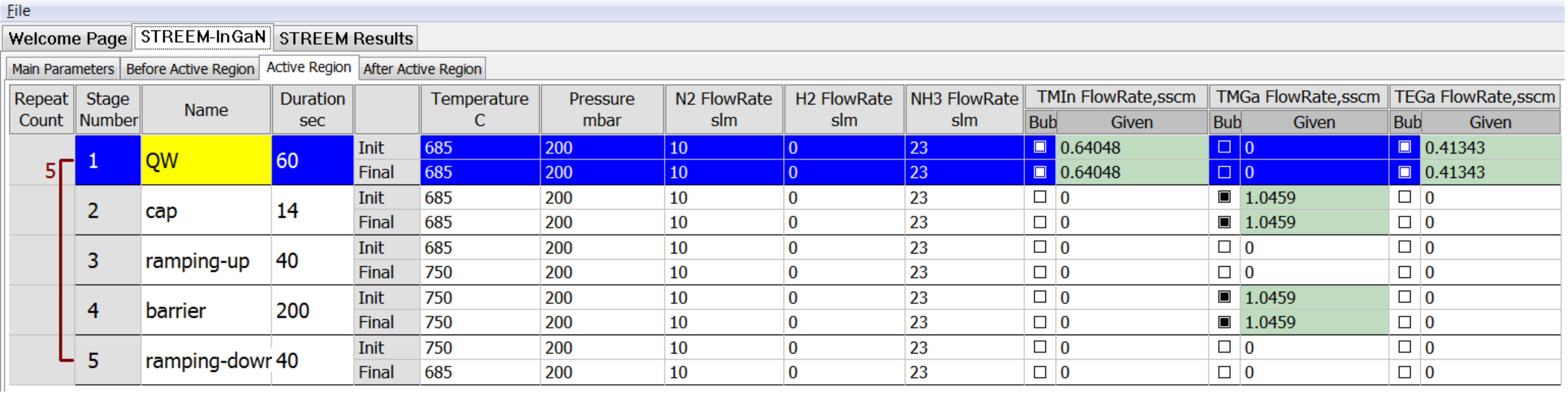
Temperature C	Pressure Torr	N2 Flow Rate slm	H2 Flow Rate slm	NH3 Flow Rat slm	TMGa Flow Rate,µ		Reference Growth Rate,µm/h
					Bub	Given	
1000	75	0	5	3	■	130,01	3

- ✓ Calibration on thick GaN growth rate: the user needs to specify only once (i) reactor type (ii) process parameters and growth rate for thick GaN – this information is normally well known.

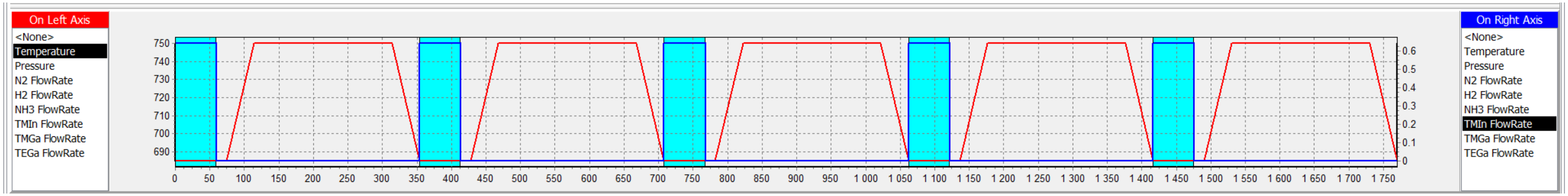
Other available options:

- ✓ Fixed diffusion layer thickness: may be used for fine tuning in case the well/barrier thickness/composition are known with high accuracy
- ✓ Average growth rate and composition may be specified for each stage in the active region

STREEM-InGaN operation: specification of the recipe

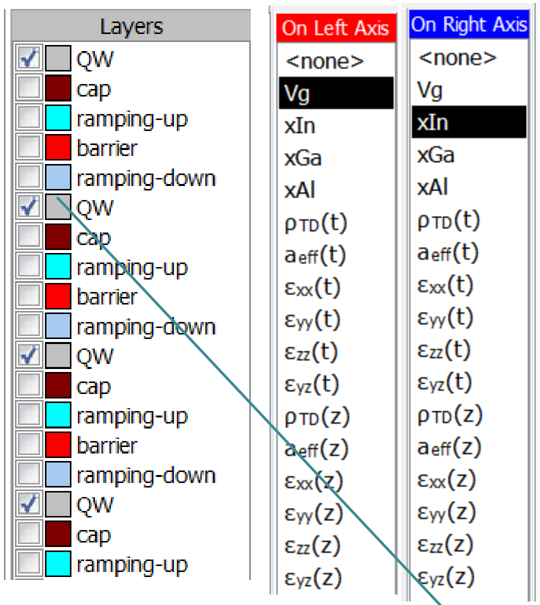


Repeat Count	Stage Number	Name	Duration sec		Temperature C	Pressure mbar	N2 FlowRate slm	H2 FlowRate slm	NH3 FlowRate slm	TMIn FlowRate,sscm Bub	TMIn FlowRate,sscm Given	TMGa FlowRate,sscm Bub	TMGa FlowRate,sscm Given	TEGa FlowRate,sscm Bub	TEGa FlowRate,sscm Given
5	1	QW	60	Init	685	200	10	0	23	☐	0.64048	☐	0	☐	0.41343
				Final	685	200	10	0	23	☐	0.64048	☐	0	☐	0.41343
	2	cap	14	Init	685	200	10	0	23	☐	0	☑	1.0459	☐	0
				Final	685	200	10	0	23	☐	0	☑	1.0459	☐	0
	3	ramping-up	40	Init	685	200	10	0	23	☐	0	☐	0	☐	0
				Final	750	200	10	0	23	☐	0	☐	0	☐	0
	4	barrier	200	Init	750	200	10	0	23	☐	0	☑	1.0459	☐	0
				Final	750	200	10	0	23	☐	0	☑	1.0459	☐	0
	5	ramping-dowr	40	Init	750	200	10	0	23	☐	0	☐	0	☐	0
				Final	685	200	10	0	23	☐	0	☐	0	☐	0



- ✓ Conventional parameters: duration, temperature, pressure, flow rates of precursors and carrier gas;
- ✓ Linear variation of process parameters within one stage is allowed;
- ✓ Ability to group several stages that are repeated more than once in the recipe;
- ✓ Graphical representation of the recipe for quick checking

STREEM-InGaN operation: visualization of the results



Layers

- ☑ ⬜ QW
- ☐ 🟫 cap
- ☐ 🟦 ramping-up
- ☐ 🟥 barrier
- ☐ 🟦 ramping-down
- ☑ ⬜ QW
- ☐ 🟫 cap
- ☐ 🟦 ramping-up
- ☐ 🟥 barrier
- ☐ 🟦 ramping-down
- ☑ ⬜ QW
- ☐ 🟫 cap
- ☐ 🟦 ramping-up
- ☐ 🟥 barrier
- ☐ 🟦 ramping-down
- ☑ ⬜ QW
- ☐ 🟫 cap
- ☐ 🟦 ramping-up

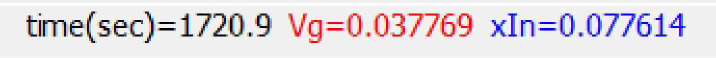
On Left Axis

- <none>
- **Vg**
- xIn
- xGa
- xAl
- $\rho_{TD}(t)$
- $a_{eff}(t)$
- $\varepsilon_{xx}(t)$
- $\varepsilon_{yy}(t)$
- $\varepsilon_{zz}(t)$
- $\varepsilon_{yz}(t)$
- $\rho_{TD}(z)$
- $a_{eff}(z)$
- $\varepsilon_{xx}(z)$
- $\varepsilon_{yy}(z)$
- $\varepsilon_{zz}(z)$
- $\varepsilon_{yz}(z)$

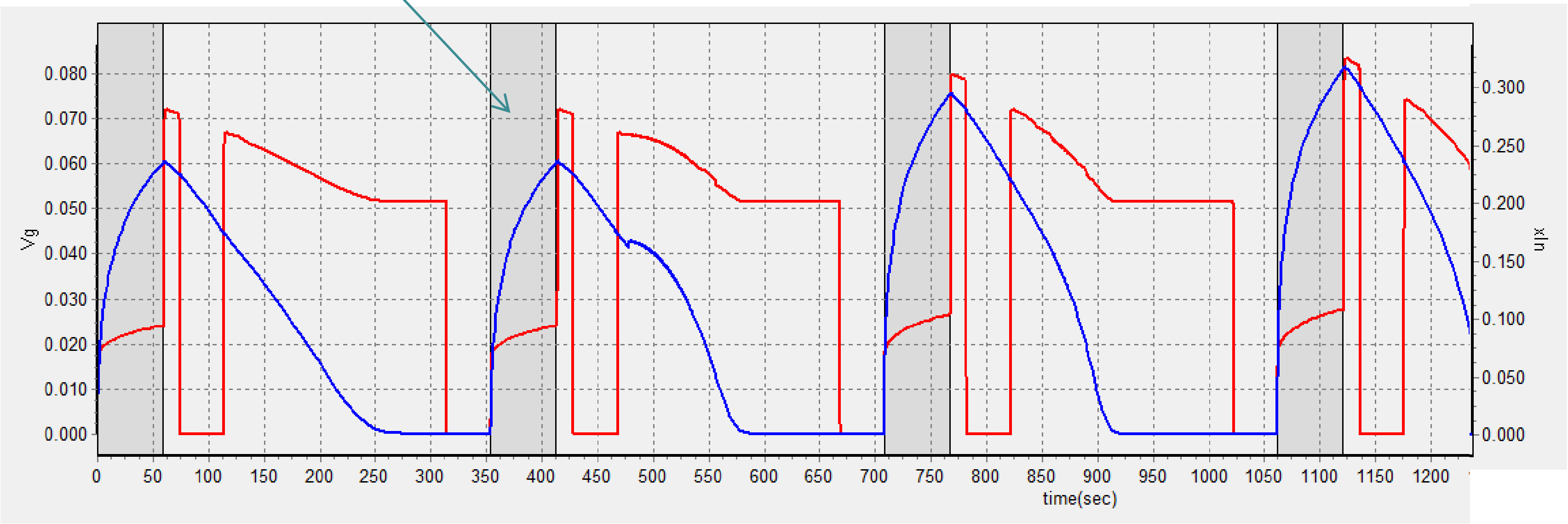
On Right Axis

- <none>
- Vg
- **xIn**
- xGa
- xAl
- $\rho_{TD}(t)$
- $a_{eff}(t)$
- $\varepsilon_{xx}(t)$
- $\varepsilon_{yy}(t)$
- $\varepsilon_{zz}(t)$
- $\varepsilon_{yz}(t)$
- $\rho_{TD}(z)$
- $a_{eff}(z)$
- $\varepsilon_{xx}(z)$
- $\varepsilon_{yy}(z)$
- $\varepsilon_{zz}(z)$
- $\varepsilon_{yz}(z)$

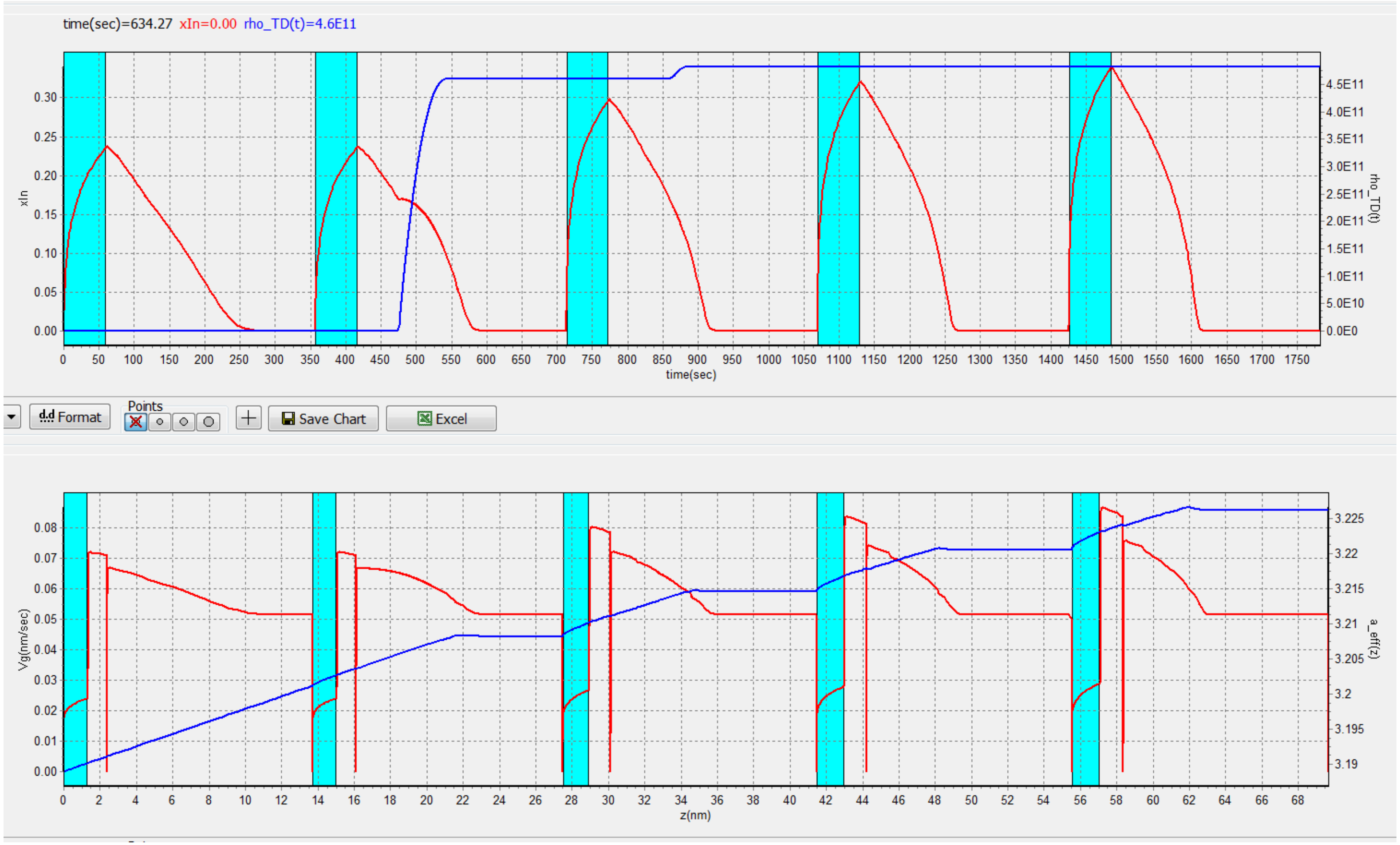
- ✓ List of process stages is available, stages with the same name are associated with a unique color;
- ✓ One or several stages can be selected to highlight them on the plot;
- ✓ Selection of the variable and its label format for the left and right axis;
- ✓ Point probe



time(sec)=1720.9 Vg=0.037769 xIn=0.077614



STREEM-InGaN operation: visualization of the results



time(sec)=634.27 xIn=0.00 rho_TD(t)=4.6E11

- ✓ growth rate, composition, effective lattice constant, dislocation density, and strain tensor components vs time and thickness
- ✓ export of the results into Excel sheet for further analysis and processing
- ✓ import of the results within SiLENSe software for the modeling of device operation

Summary

STREEM-InGaN may be used to analyze:

- influence of the process parameters on indium incorporation into the quantum wells;
- composition profile in the active region of the heterostructure;
- strain distribution in the active region by both modifying the operating parameters and modifying the structure;
- onset of stress relaxation via formation of dislocations;
- evolution of the composition, strain, and dislocation density