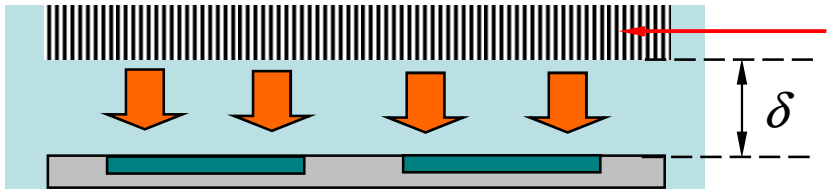
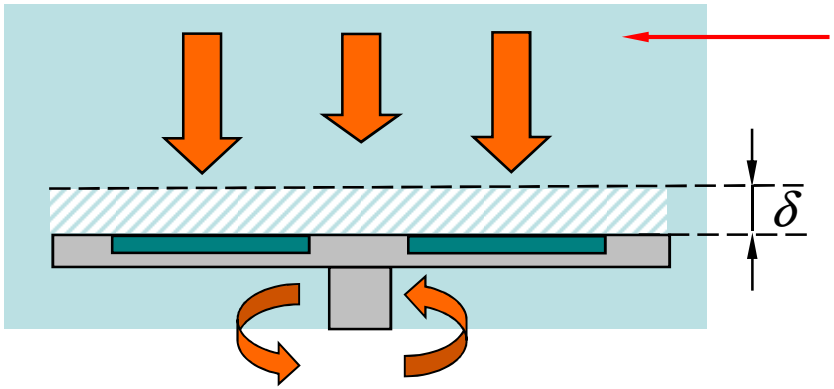
Diffusion boundary layer in typical MOCVD reactors



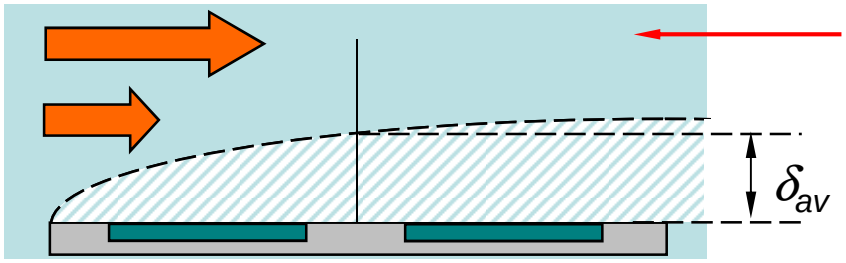
Close Coupled Showerhead

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



Rotating Disk Reactor

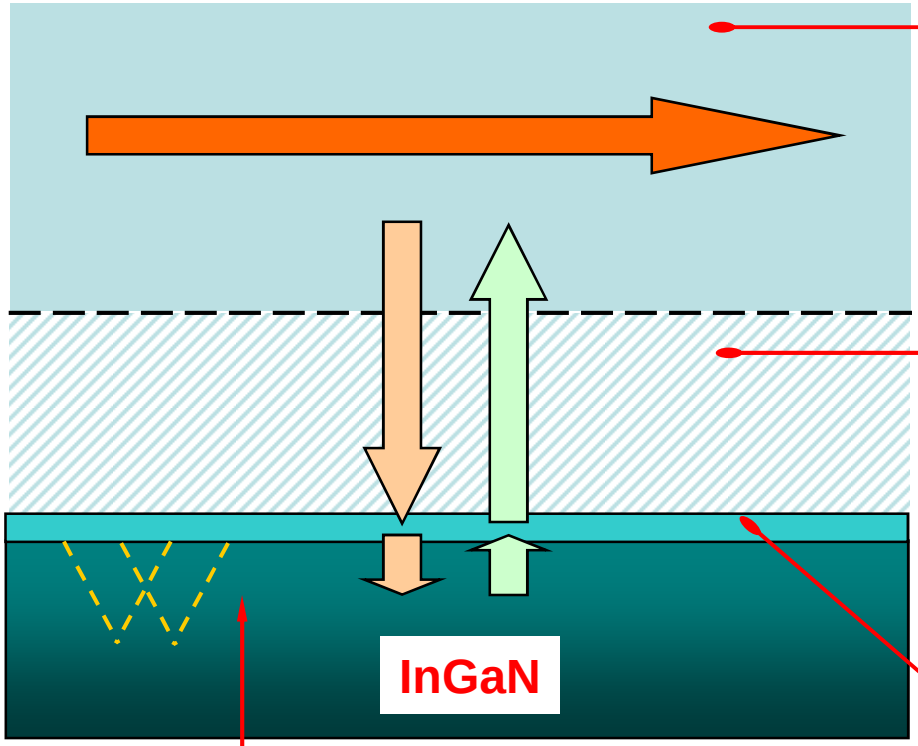
- Narrow rotation boundary layer is formed due to the dominant susceptor rotation



Horizontal/Planetary Reactor

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

Approach to unsteady modeling of InGaN/GaN MOCVD



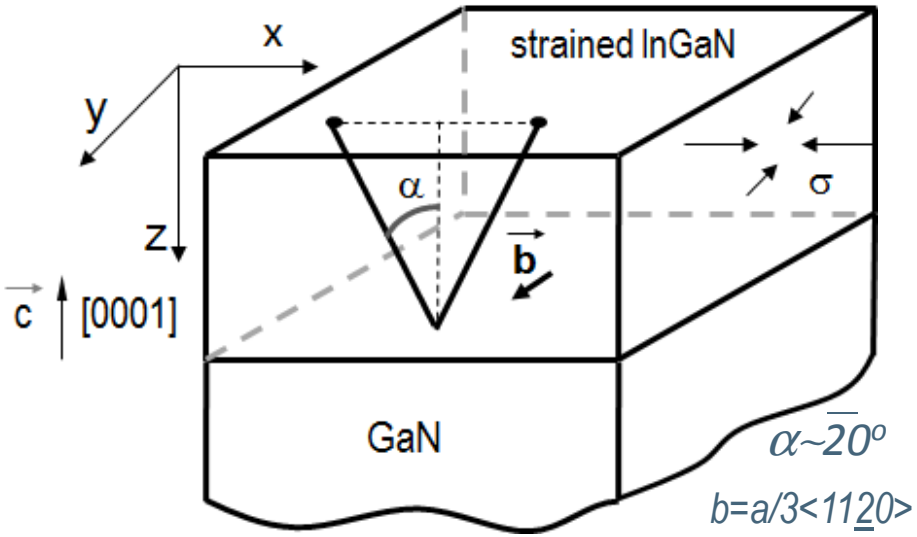
Gas flow core
- Unsteady supply of precursors TMIn, TMGa, TEGa, and NH_3 with carrier N_2 and H_2

Diffusion boundary layer
- Diffusion transport of gas species to/from the interface

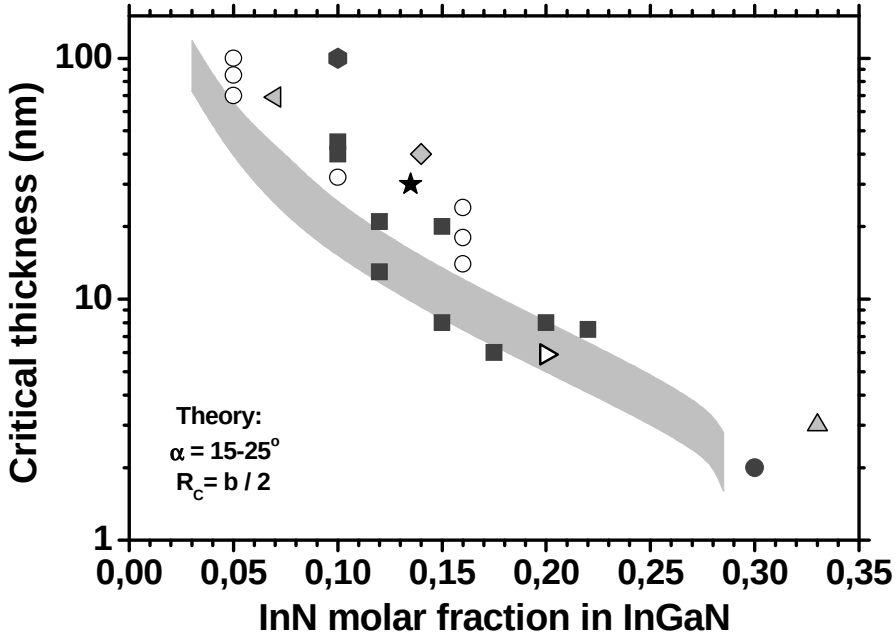
Adsorbed layer
- Unsteady balance of adsorbed atoms In, Ga, N, and H
- Mass exchange with gas (adsorption/desorption)
- Mass exchange with crystal (incorporation/decomposition)

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

STREEM-InGaN 2.0 | C:₩Program Files (x86)₩STR IP Holding₩STREEM-InGaN Edition 2.0₩Examples₩Example6₩Lekhal_APL_2015_A3.stm

File

Welcome Page | STREEM-InGaN | STREEM Results

Main Parameters | Before Active Region | Active Region | After Active Region

1. "No Relaxation: is pseudomorphically grown on the underlying layer (GaN by default).
2. "V-dislocations": Stress relaxation in the InGaAlN/GaN active region via formation of V-shaped dislocation half-loops is considered.
3. only the growth rate of the layers in the before(n-GaN) and after active region(p-GaN) is automatically caculated. other units is not automatically caculated.
4. "Standard": ignoring surface site blocking with adsorbed indium
5. "Site Blocking": considering surface site blocking with adsorbed indium
6. "No segregation": the nominal composition profile without 'In' segregation
7. "Reference Growth Rate, um/h": is used to estimate the boundary layer thickness at the stage of thick GaN growth.
   User can input the average growth rate of thick GaN layer in user's reactor configuration.

Main Parameters

Relaxation Model
1. ○ No relaxation
2. ◉ V-dislocations

Units
Temperature: C
Pressure: Torr
3. Growth Rate: µm/h
Group III Flow Rate: µmol/min

Segregation Model
4. ○ Standard
5. ◉ Site Blocking
6. ○ No Segregation

Reactor Transport Model
A. ○ Fixed diffusion layer thickness
B. ◉ Calibration on thick GaN layer growth rate
C. ○ Calibration on average 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 Rate slm	TMGa Flow Rate,µmol/min		7. Reference Growth Rate,µm/h
					Bub.	Given	
1000	75	0	5	3	■	130.01	3

A.: to specify directly the boundary layer thickness for each stage in the active region ==>For fine tunning in case the well/barrier thickness/composition are known with high accuracy!

B.: Since the boundary layer thickness is computed differently for different reactor types.

C.: To have to specify an average growth rate and composition for each layer in the active region.

STREEM utilizes the partial GaN growth rate [Vg_{GaN}~(1-X_{In})*Vg_{InGaN}]

==> Should be specified for each stage in the active region

Run Solver | F Font

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File

Welcome Page | STREEM-InGaN | STREEM Results

Main Parameters | Before Active Region | Active Region | After Active Region | (p-GaN)

Repeat Count	(n-GaN) Stage Number	Name	Thickness characteristics						Composition 1.						Dislocation density 1/cm²		2. Stress state			
			Thickness,nm		Duration,sec		Growth rate,μm/h		AlN		GaN		InN							
			Calc	Given	Calc	Given	Calc	Given	Calc	Given	Calc	Given	Calc	Given	Inheri	Given	Used	a,Å	Used	Relax.Degree
	1	n-GaN	○	10	○	540	◉	0.066667	◉	0	○	1	○	0	☐	1e+9	◉	3.189	○	

"Before Active region"(n-GaN) and "After Active region"(p-GaN) 탭의 입력 방법

1. Dislocation density: n-GaN의 첫번째 layer에서 반드시 정의해야함, 그리고 이후 layers에서는 상속(inherit) 선택 하거나 측정값이 있을 경우 직접 입력함

2. Stress state: lattice mismatch와 strain 계산시 이값을 부차적으로 사용하기 위해서 Active region아래에 있는 layer의 lattice constant를 정의해야함
   - Lattice constant: AlN(3.112A), GaN(3.189A), InN(3.54A)
   - Relaxation degree: '1': 직전 layer의 격자상수와 현재의 layer의 격자상수가 같다는 의미
     a(eff./current)-a(eff./previous)=a(bulk/current)-a(eff./previous), a(bulk):fully relaxed를 의미함

참고,: Before/After Active region 탭을 입력하지 않는 경우 "The Active region"은 Thick relaxed GaN위에 성장되는 것으로 가정함.

Repeat Count | Append <Ctrl+Enter> | Delete | Insert Before | Insert After | Move Up | Move Down | Copy | Paste | Export to Excel | Run Solver | Font

STREEM-InGaN 2.0 | C:₩Program Files (x86)₩STR IP Holding₩STREEM-InGaN Edition 2.0₩Examples₩Example6₩Lekhal_APL_2015_A3.stm

File

Welcome Page | **STREEM-InGaN** | **STREEM Results**

Main Parameters | Before Active Region | Active Region | After Active Region

Repeat Count	Stage Number	Name	Duration sec		Temperature C	Pressure Torr	N2 FlowRate slm	H2 FlowRate slm	NH3 FlowRate slm	TMIn FlowRate,µmol/m		TMGa FlowRate,µmol/m		TEGa FlowRate,µmol/m		TMAl FlowRate,µmol/m	
										Bub.	Given	Bub.	Given	Bub.	Given	Bub.	Given
10	1	QW	135	Init	715	350	4	0	4	☐	2.3266	☐	6,0037	☐	0	☐	0
				Final	715	350	4	0	4	☐	2.3266	☐	6,0037	☐	0	☐	0
	2	GaN cap	180	Init	715	350	4	0	4	☐	0	■	6,0037	☐	0	☐	0
				Final	715	350	4	0	4	☐	0	■	6,0037	☐	0	☐	0
	3	Ramping	100	Init	715	350	4	0	4	☐	0	☐	0	☐	0	☐	0
				Final	940	350	4	0	4	☐	0	☐	0	☐	0	☐	0
	4	AlGaN barrier	477	Init	940	350	4	0	4	☐	0	■	6,0037	☐	0	☐	1.37
				Final	940	350	4	0	4	☐	0	■	6,0037	☐	0	☐	1.37
	5	GaN barrier	390	Init	940	350	4	0	4	☐	0	■	6,0037	☐	0	☐	0
				Final	940	350	4	0	4	☐	0	■	6,0037	☐	0	☐	0
	6	Ramping	100	Init	940	350	4	0	4	☐	0	☐	0	☐	0	☐	0
				Final	715	350	4	0	4	☐	0	☐	0	☐	0	☐	0

_Modeling of the stress and compsotion profile is actually performed for the active region, so thick InGaN layer or superlattice can be considered in the "Active region" tab.

-복수선택: "Shift +left mouse"

-반복을 원하는 레이어들을 "shift+left mouse"클릭-->"Repeat count"클릭 --->반복횟수 입력

-Copy명령 실행시 Stage name은 복사되지 않고 공란으로 처리됨

-Process parameter 입력시 stepwise(계단형)형태의 변화를 피하고 slope을 주어 입력함(리액터 inlet에서의 gas composition의 stepwise 변화가 있더라도 growth 표면에서는 gas species interfusion때문에 smoothe 해지기 때문)!

예를들면, 사용자 가이드 Fig.7.3 참고

"Relaxation Model" option과 dislocation density입력

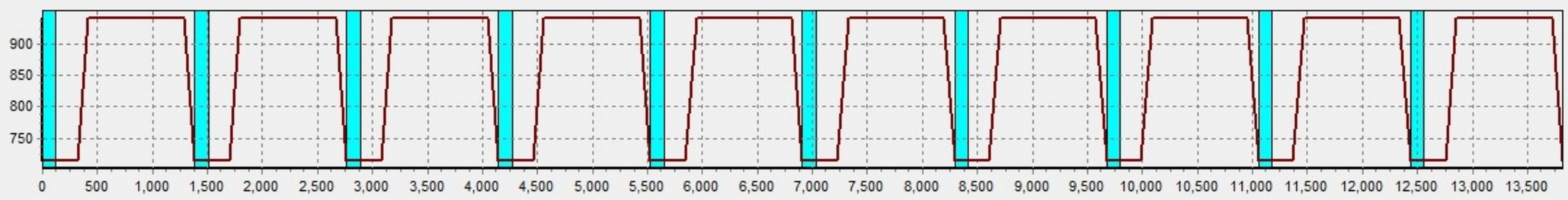
-"main paramters"탭에서 "V-shaped dislocation"을 선택한 경우, active region의 dislocation density가 자동으로 계산되기 때문에 입력할 필요가 없음

-"main paramters"탭에서 "No Relaxation" 이 선택된 경우 active region 탭의 모든 layer에 직접 입력하거나 이전 layer에서 상속 받아야함.

- 만약, Before Active region(n-GaN)탭에서 어떤 layer도 정의되지 않았다면 Active region의 첫번째 layer에서 dislocation density를 정의해야함

참고: "No Relaxation" 선택시 Composition profile 계산에는 영향을 주지 않고 , SiLENSe에서 STREEM 결과값을 import시 dislocation density 값으로 사용됨

On Left Axis: <None> | Temperature | Pressure | N2 FlowRate | H2 FlowRate | NH3 FlowRate | TMIn FlowRate | TMGa FlowRat



On Right Axis: <None> | Temperature | Pressure | N2 FlowRate | H2 FlowRate | NH3 FlowRate | TMIn FlowRate | TMGa FlowRat

Repeat Count | Append <Ctrl+Enter> | Delete | Insert Before | Insert After | Move Up | Move Down | Copy | Paste | Export to Excel | Run Solver | Font