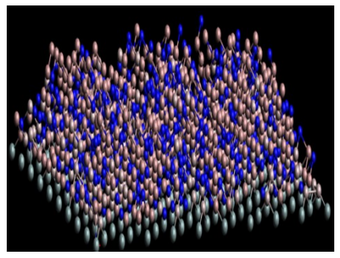
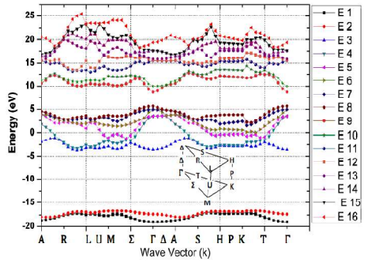
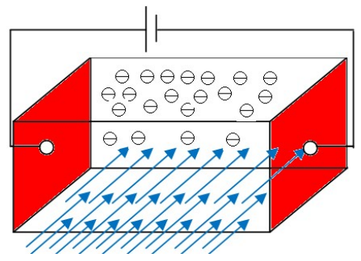
Horizontal MOCVD Injector Reactor

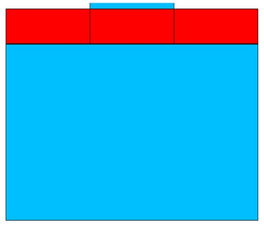
TNL- Injector Simulator

Technology of Next Level
driven through innovation









CHALLENGES: MOCVD EPITAXY

- ❑ MOCVD ➡ *Chemical process* to deposit special materials and high-tech devices
- ❑ Growth mechanism Investigation of III–V compounds ➡ *High value products*
- ❑ Film growth properties, closely related to product quality ➡ Depends gas *inlet flow rate*, *operating pressure & temperature* and *reactor geometry configurations*
- ❑ High-quality demands of the semiconductor industry ➡ control composition distributions in a MOCVD reactor to achieve *film growth thickness* & *uniformity*
- ❑ MOCVD : *complex transport phenomena* ➡ momentum, heat, mass & chemical reactions
- ❑ MOCVD reactor's optimal growth condition ➡ requires extra experimentation to refine & search process to locate an optimal solution until film deposition quality satisfies a pre-specified criteria.
- ❑ Two categories: ➡ Development of a chemical kinetic & Transport phenomenon
- ❑ To save design cost & development time ➡ use of *CAD methodologies* of MOCVD processes.

Challenges: GaN/Si Epitaxy

- ❑ *GaN directly on Si* encounters several challenges → large lattice mismatch (*16% to 20.4%*) and thermal expansion coefficient (*TEC*) mismatch ~ *53%* leads to the generation of defects at room temperature
- ❑ *AlN buffer layer* growth prior to the growth of GaN → To *avoid formation of cracks* and several *other technological challenges*
- ❑ *Stack of $Al_xGa_{1-x}N$ layers* on AlN buffer layer → *To balance compressive and tensile strain*
- ❑ Growth of the AlN buffer layer on the Si substrate → *Still not well understood*
- ❑ Well known phenomenon of formation of *amorphous SiNx*, deteriorates crystalline quality.
- ❑ Pre-nitridation process of Si substrate greatly influences surface morphology. However, nitridation time and substrate nitridation temperature highly influence strain generation between each layer and results in defect formation process
- ❑ NH_3 pre-flow with smaller step size time and the optimum substrate temperature are still ***debatable*** to achieve a single-crystalline GaN on Si substrate

Challenges: GaN/Si Epitaxy

- GaN-on-Si devices recently attracted much attention *for radio frequency* (RF) applications due to *cost & large size Si substrates* with possibility *of co-processing in CMOS foundries*
- However, GaN-on-Si RF devices, still facing some challenges in form of ***RF loss***
- Contributor to RF loss is *parasitic channel formation* at AlN/Si interface
- Type of conductivity & formation mechanism of parasitic channel is ***controversial***
- Few groups suggest formation of a p-type conductive layer at the AlN/Si interface, while others suggest that an n-type electron channel induced by the strong polarization field at the AlN/Si interface.
- Understanding the behaviors of the parasitic layer is crucial for reducing the RF loss
- Unsolved problem requires an unambiguous identification of this conductive layer and correlating it with the RF loss

AVAILABLE SOLUTION

❑ Numerical simulations, (*CFD software) ONLY* predicts ➡ Film growth rate and uniformity, Prediction accuracy heavily relies on the reaction kinetics mechanism, however, transport phenomena oversimplified *by assuming constant mass diffusivity for precursors, temperature-independent properties of gas mixture*, and *constant wall temperature profile or constant heat transfer coefficient for boundary condition of inner reactor wall*.

❑ ***Oversimplifications*** made for the heat transfer ➡ substantially prohibit the prediction ability of the MOCVD processes, making a great discrepancy between the model and the actual behavior of the film growth on substrate.

❑ To extract atomistic scale information of MOCVD reactor process through CFD software is **IMPOSSIBLE**

EPITAXY PROCESS SOLUTION

Innovative Atomistic Scale Reactor Simulation without use of Continuum models

TNL Framework

- MBE Reactor Process
- CVD Reactor Process
- PECVD Reactor Process
- MOCVD Reactor Process (Vertical Precursors Flow)
- MOCVD Reactor Process (Horizontal Precursors Flow)

- User's Input Growth Conditions
- Surface Profile (Roughness)
- Strain Mapping (layer by Layer
- Lattice parameter
- Defects (Vacancies, Interstitials, Dislocations, Stacking Faults)

INPUTS : MOCVD PROCESS

Chamber Condition

☐ **Showerhead Based**

☑ **Injector Based**

Injector Parameters

Chamber Volume (ltrs.)	1.4	
Chamber Pressure	10	torr
Ceiling Height (cm)	2.0	
Chamber Temperature (C)	100	
Sticking Coeff.	1	

Many More parameters details Require …….

Precurssor Condition

Number of Port: 0

Precursor 1: Select Prec...

Flow Rate: atm cc/s

Load Reaction | Step 1 | Load 1

Precurssor Condition

Number of Port: 4

Precursor 1: Select Prec...

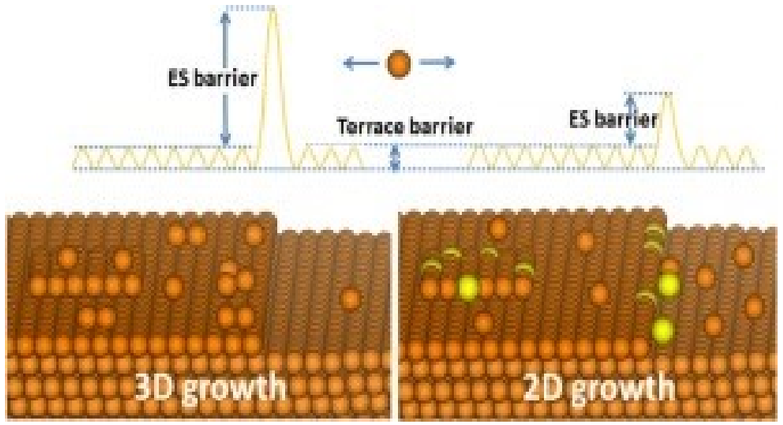
Flow Rate: m cc/s

Load Reaction | Load 1

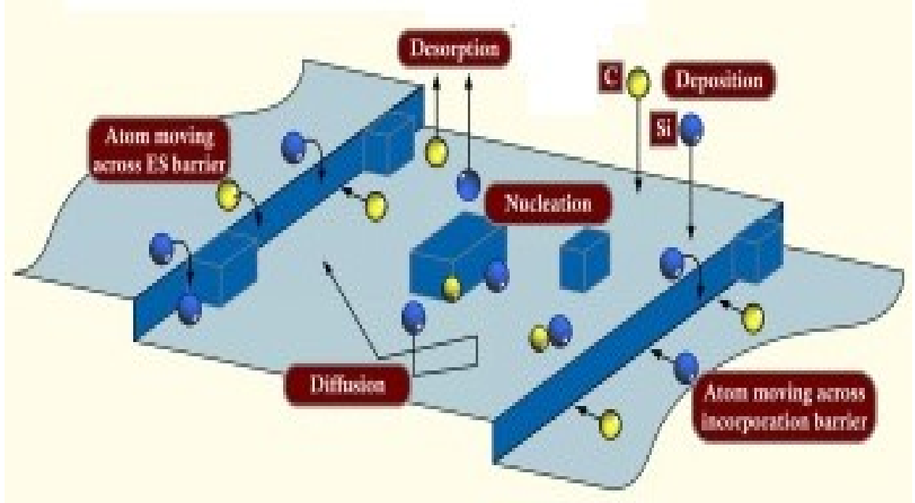
- Select Precursc
- Ga(CH3)3
- (CH3)3CAsH2
- H2
- Al(CH3)3
- NH3
- CH3
- O2

METHODOLOGY: MOCVD PROCESS

Schwoebel barrier: The atom diffuses from the site exactly above the edge atom to the site immediately next to the edge atom as;



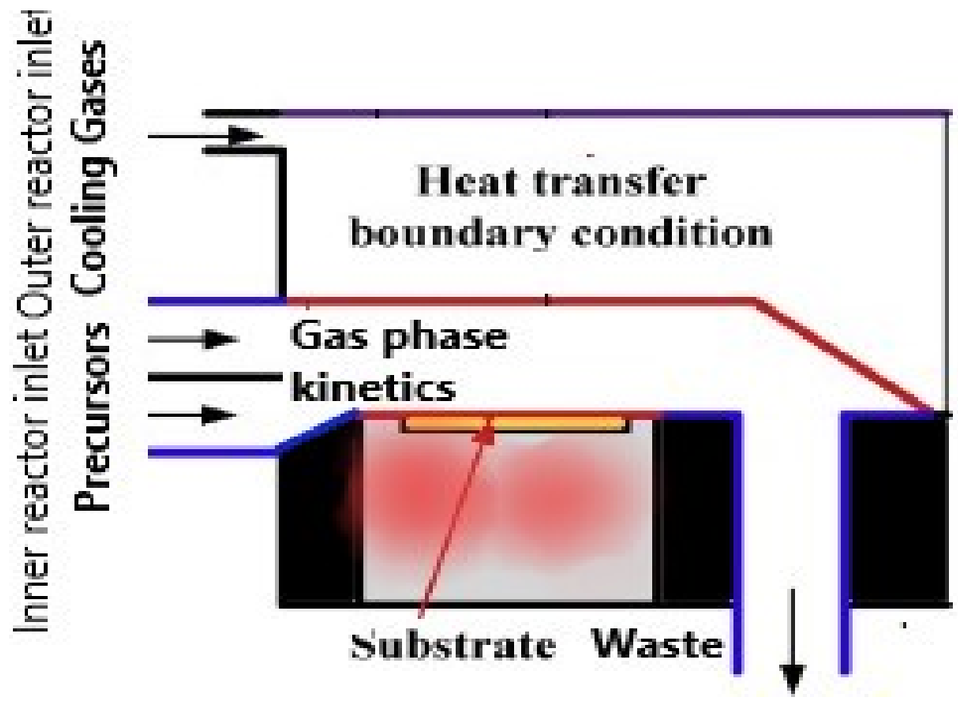
Incorporation barrier: The atom incorporates into the edge on the same surface level.



PLANETARY MOCVD PROCESS

Planetary MOCVD architecture implemented in ***TNL-Injector*** **simulator** equivalent to the **AIX 200/4 horizontal MOCVD reactor**.

Inlet of the reactor is divided into two parts by a separator through which the group III and V precursors can be fed into the upper and lower inlet respectively.



PLANETARY MOCVD PROCESS

The reactant flux, $J_A = -\frac{D_{AB}}{RT}\frac{dc_A}{dx}$ with $\frac{dc_A}{dx} \approx \frac{\Delta c_A}{\Delta x} = \frac{c_{AB} - c_{AS}}{\delta}$

where J_A is the diffusion flux of specie A, is the concentration of species A, x is the direction perpendicular to the substrate surface, *R* is the gas constant, *T* is the absolutc$_A$ e temperature. δ is the chamber boundary layer thickness.

D_{AB} is the diffusivity of the bulk stream reactants and dependent on Leonard-Jones parameters (σ, Ω) based on the Chapman-Enskog theory

$$D_{AB} = 2.7 \times 10^{-3} \frac{\sqrt{T^3\left(\frac{1}{M_A} + \frac{1}{M_B}\right)}}{p\sigma_{AB}^2 \Omega_{D,AB}}$$

M is the molecular weight, p is the pressure, σ_{AB} is the collision diameter, and Ω_D, AB is the collision integral and dependent on temperature and intermolecular potential.

Average boundary layer thickness, δ, $\bar{\delta} = \frac{10}{3}\sqrt{\frac{\mu_{mix} L}{\rho U}}$

PLANETARY MOCVD PROCESS

An Injector MOCVD reaction initiate either surface kinetic or mass transport control. Suppose C_g is the concentration of the bulk gas and C_s is the concentration of reactants at the substrate interface. The concentration of the reactants drops from the bulk to the substrate surface and the corresponding mass flux,

$$I_{gs} = h_g(C_g - C_s)$$

where h_g is the gas mass transfer coefficient, insensitive to variations in temperature.

The flux consumed at the surface $I_s = k_s(C_s)$ where $C_s = \frac{C_g}{1+\frac{k_s}{h_g}}$

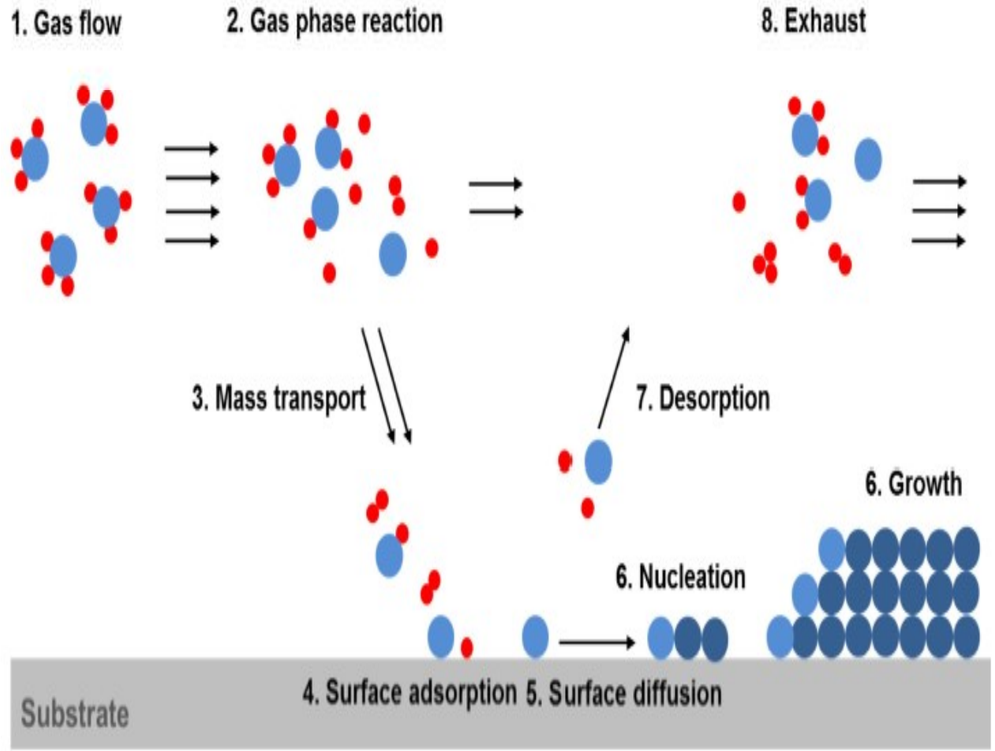
where k_s is the slowest surface reaction rate constant.

For $\boldsymbol{k_s >> h_g}$, the system dictated by mass controlled , low gas transport rate through the boundary layer limits the rapid surface reaction.

Surface reaction control dominates for $\boldsymbol{h_g >> k_s}$, the surface reaction is slow even through sufficient reactant gas is available. Additionally, h_g increases with increasing pressure and decreasing temperature and k_s follows the Arrhenius equation.

WORKING

- ❖ Gas phase kinetics
- ❖ Surface phase kinetics
- ❖ Each monolayer with atoms positions
- ❖ Defects layer by layer quantitatively and qualitatively
- ❖ Strain layer by layer
- ❖ Surface Roughness
- ❖ Lattice Constant etc.



TNL Chemical Database

Precursors for MN Growth

(M = Ga, Al, In)

1. TMM
2. DMM
3. NH_3
4. N_2

Dopants

1. Cp2 Mg
2. Silane

Carrier Gases: MN Growth

1. N_2
2. H_2
3. Ar

$$A + B \leftrightarrow AB$$

$$\frac{d[AB]}{dt} = \frac{k_1[A][B]^2}{1 + k_2[A] + k_3[B]^{1/2}}$$

Reaction rates in forward and reverse directions

$$k = AT^n \exp\left(-\frac{E_a}{RT}\right)$$

KINETIC MONTE CARLO (KMC)

Total Deposition Rate:

$$R = A + H + D$$

A - Adsorption, H – Diffusion, D - Desorption rates

$A = Flw$ Here, l and w denote length and width of substrate

$h_j = D_0 exp\left(-\frac{E_j}{k_B T}\right)$ The characteristic vibration frequency , $D_0 = \frac{2k_B T}{h}$

$d_j = D_0 exp\left(-\frac{E_j^{des}}{k_B T}\right)$ with $E_j^{des} = E_S + nE_n$

EXTRACTABLE

1. Lattice Parameters:

- ❑ Layer by layer lattice parameter Extraction.
- ❑ Averaging layer by layer lattice constant may produce overall lattice constant of film.
- ❑ The lattice constant can be calibrated with lattice constant with XRD studies.
- ❑ Lattice constant includes all the strain, defects etc effects.

2. Strain:

- ❑ Averaging layer by layer strain produce overall strain in the film.
- ❑ The strain can be calibrated with experimental strain.

3. Surface Roughness:

- ❑ Extract surface roughness as a function of growth time

$$r = \sqrt{\frac{\sum_{i=1}^{N}\sum_{j=1}^{N}[h_{ij}-\bar{h}]^2}{NxN}}$$

Here N is the total number of lattice points, h_{ij} is the height at a given lattice point located at position *i* and *j*, on the lattice and h_{avg} is the average height of all lattice points.

4. Mole fraction:

- ❑ Extract number of atoms of different constituents layer by layer.
- ❑ Ratio of group-III & V deposited atoms ➡ Molefraction.

5. Defects :

- ❑ Extract number of interstitials, vacancy etc layer by layer along with dislocation and Stacking Faults

Case Study : **Si/AlN** Planetary MOCVD Process

INPUT CONDITIONS

Parameters	Si/AlN	Pre-Nitridated Si/AlN
Chamber Temperature (°C)	300	300
Chamber Pressure (mbar)	40	40
Chamber Volume (lits)	1.4	1.4
Ceiling Height (cm)	1	1
Substrate Temperature (°C)	1050	1050
Precursors	TMAl & NH_3	TMAl & NH_3
Precursors Flow Rate (sccm)	105 sccm & 1 slm	105 sccm & 1 slm
Carrier Gas	H_2	H_2
PreNitridation(slm)	-	1

Parameters	Si/AlN	Pre-Nitridated Si/AlN
Nitridation Temperature (C)	-	1050
Nitridation Time (s)	-	30
Surface Energy (eV)	2.0	2.0
Desorption Barrier (eV)	3.0	3.0
Schwoebel Barrier (eV)	0.05	0.05
Incorporation Barrier (eV)	0.05	0.05
Nearest Neighbour (eV)	0.05	0.05
No. of Interactive Elements	1	1
Substrate Dimension (A^2)	50x50 [Unit Cell]^2	

CHEMICAL KINETICS

Gas Phase Equations

Al(CH3)3 = AlCH3 + 2CH3 ,	A=3.5*10^15,	n=0,	Ea= 66500
Al(CH3)3 + NH3 = Al(CH3)3:NH3 ,	A=3.0*10^12	n=0	Ea= 0.0
Al(CH3)3:NH3 = Al(CH3)3 + NH3 ,	A=5.0*10^10	n=0	Ea= 22000
Al(CH3)3:NH3 = (CH3)2Al:NH2 + CH4 ,	A=2.0*10^12	n=0	Ea= 27000
Al(CH3)3:NH3 + NH3 = (CH3)2Al:NH2 + CH4 + NH3 ,	A=2.0*10^12	n=0	Ea= 13000
2(CH3)2Al:NH2 = ((CH3)2Al:NH2)2 ,	A=4.0*10^11	n=0	Ea= 0.0

##Gas to Surface Phase Equations

Al(CH3)3 + space = Al(S) + 3CH3 , coll 1.0

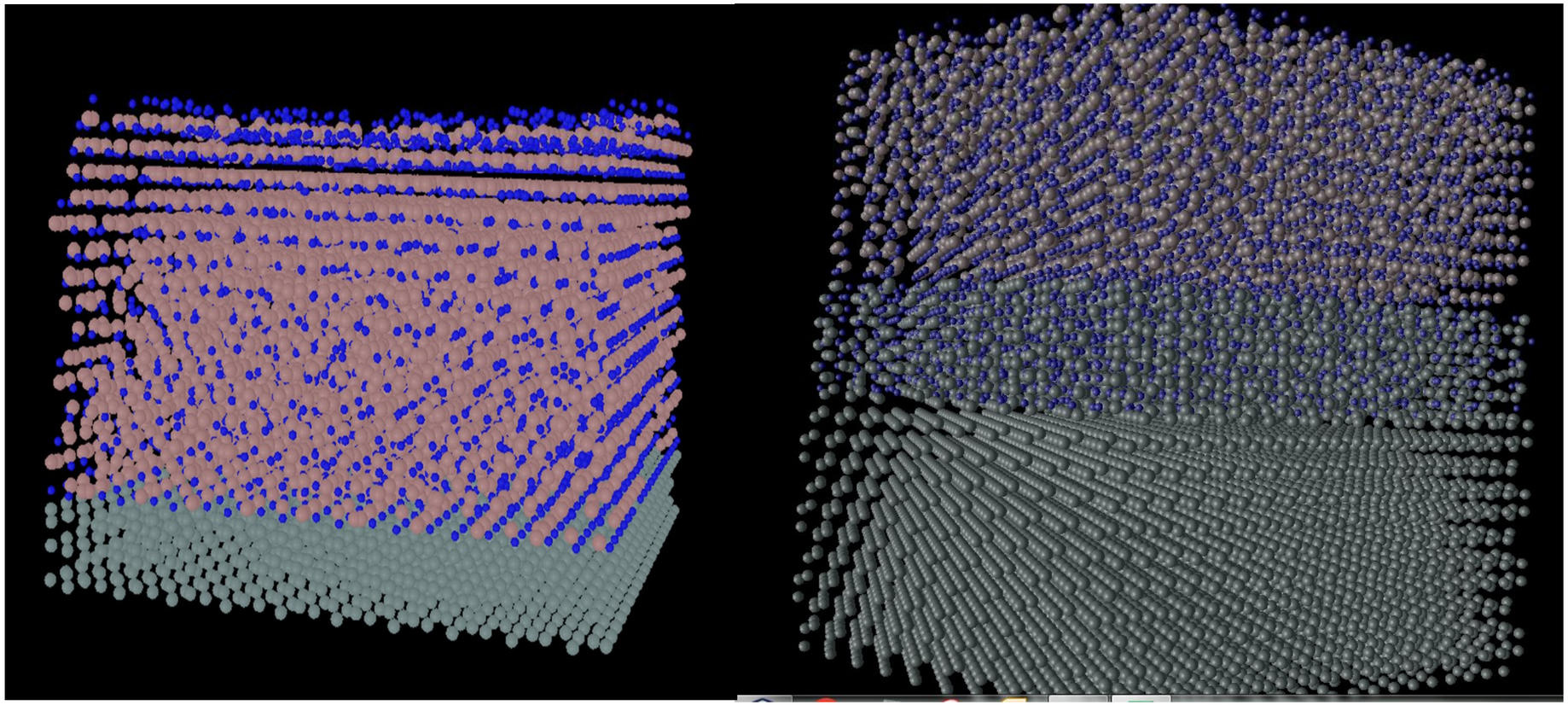
Al(CH3)3:NH3 + space = Al(S) + 3CH3 + NH3 , coll 1.0

AlCH3 + space = Al(S) + CH3 , coll 1.0

(CH3)2Al:NH2 + space = AlN(S) + 2CH4 , coll 1.0

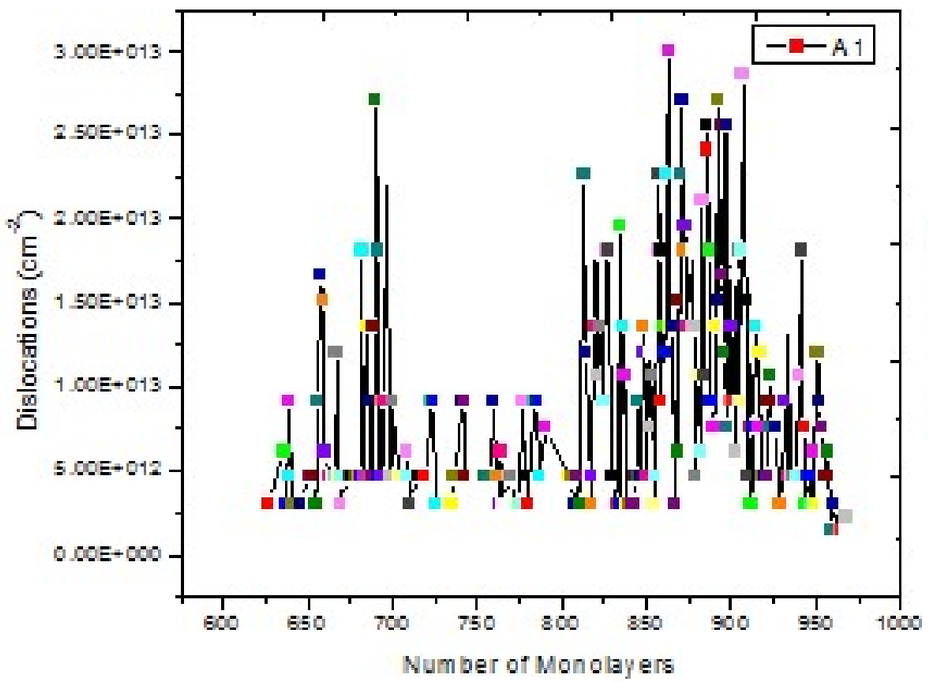
((CH3)2Al:NH2)2 + space = 2AlN(S) + 4CH4 , coll 1.0

OUTPUT

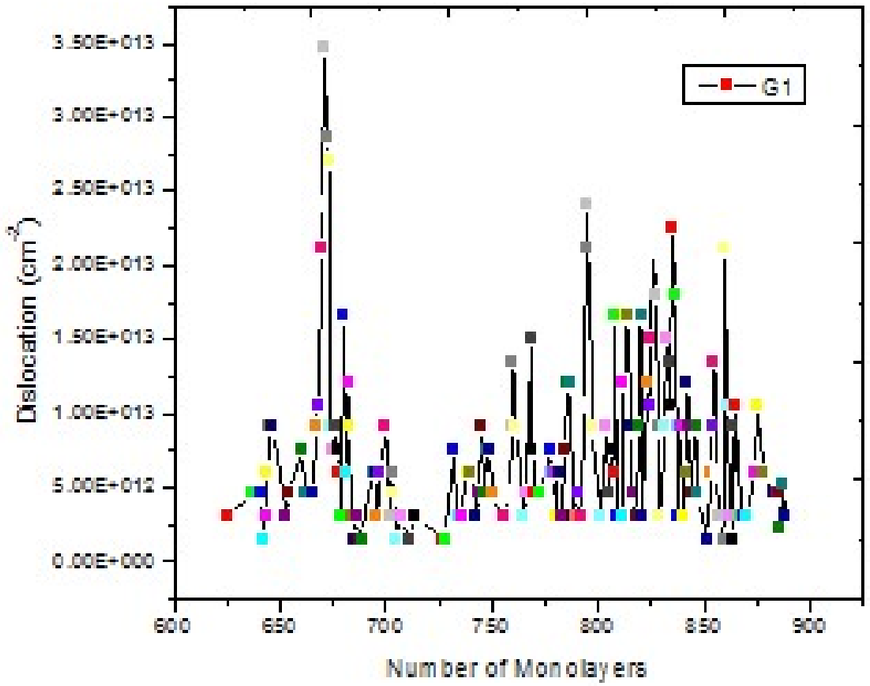


Without Nitridation **Pre-Nitridation for 30 s**

Dislocations Per Monolayer

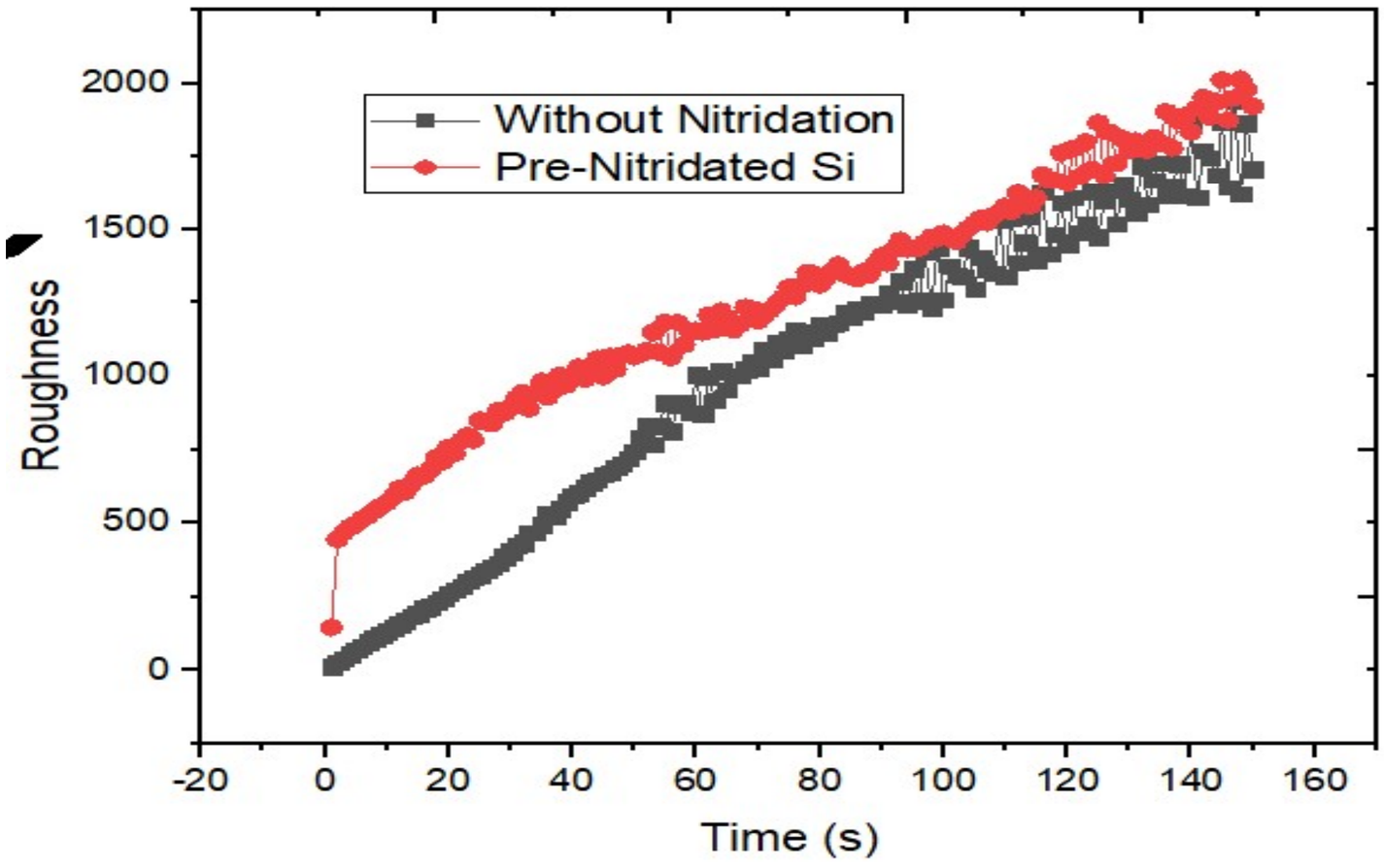


Without Nitridation



Pre-Nitridation for 30 s

Surface Roughness



Other Output

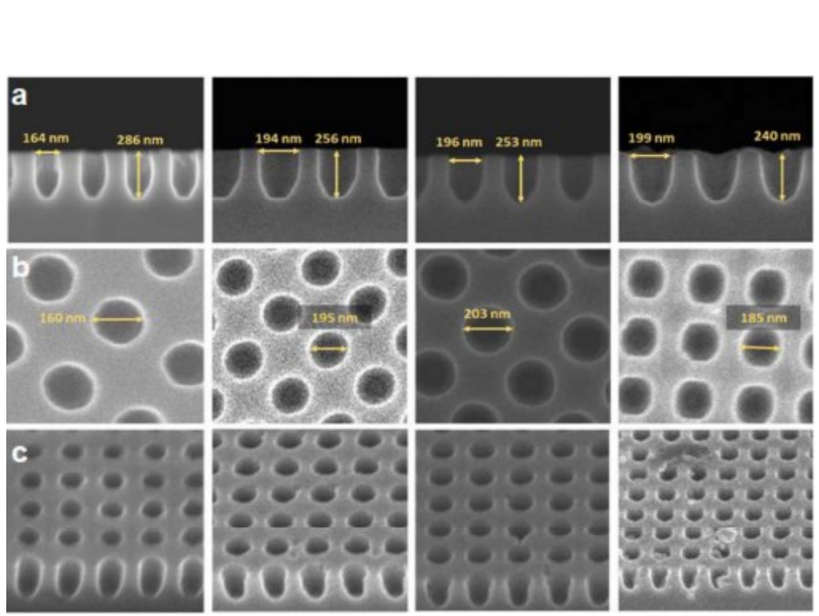
Parameters	Si/AlN	Pre-Nitridated Si /AlN
Substrate Thickness (µm)	0.3258	0.3258
Si3N4 Thickness (nm)	-	3.7817
Total Deposited Atoms (AlN)	5046178	5233815
Vacancies (cm^{-3})	36069	13393
Total Dislocation Density (cm^{-3})	2503	1612
Al Atoms	≈50%	≈50%
N Atoms	≈50%	≈50%
Many More ……		

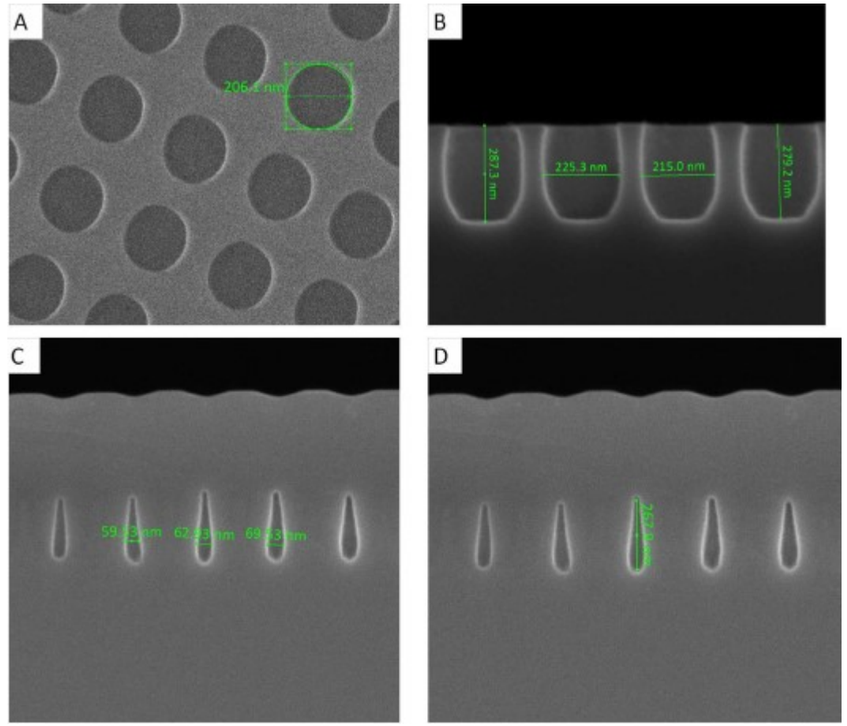
Patterned Substrate: Selective Epitaxy

TNL-Injector Simulator provides flexibilities to simulate regrowth processes at Atomistic Scale for Selective Epitaxy with capabilities:

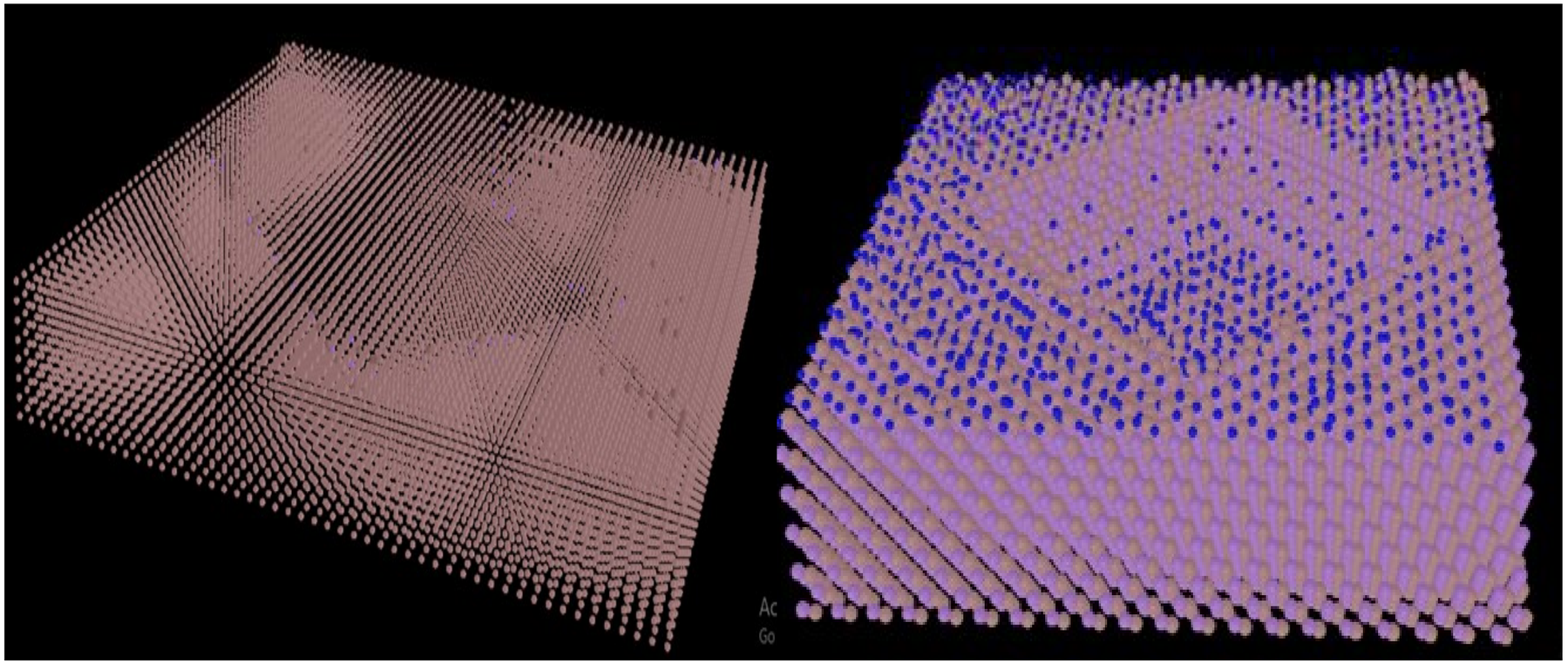
- *Process* Optimization
- Atomistic growth process for void-semiconductor photonic crystal (PhC)
- Better understanding of invisible *Physical Phenomenon*
- *Patterned substrates Shapes: Steps, Grooves, Well etc.*
- *Epitaxial growth through: MBE, MOVPE/MOCVD*
- *Effects of regrowth on **air-hole morphology***
- Comparison between patterned substrate hole regrown void's dimensions
- patterned substrate hole: *play a very critical role in the final regrowth*
- *Many More Benefits ….*

MAJOR CHALLENGES: DIMENSIONS OF AIR HOLE





Re-growth over Step Patterned Substrate



Regrowth of Si over GaAs Step Pattern Substrate Unit Cells representation

Regrowth of Si over GaAs Step Pattern Substrate Atomistic representation

ADVANCE LICENSING & PRICE VALUE

TNL's tools support advanced and unique licensing models tailored for unique customer needs.

➢ ADVANCED LICENSING OPTIONS:

- Term-Based
- Perpetual with Annual Maintenance Cost (AMC)
- TCAD Academic Suite
- 24x7 Technical Support for **Academic Institutions**

Publications

1. P.K. Saxena, numerical study of dual band (MW/LW) ir detector for Performance improvement, *Defence Science Journal*, vol. 67(2), (2017) pp. 141-148. DOI : 10.14429/dsj.67.11177
2. Praveen K. Saxena, Pankaj Srivastava, R. Trigunayat, An innovative approach for controlled epitaxial growth of GaAs in real MOCVD reactor environment, *Journal of Alloys and Compounds, vol.* 809 (2019) 151752. https://doi.org/10.1016/j.jallcom.2019.151752
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6. A. Srivastava, A. Saxena, P. K. Saxena, F. K.Gupta, P. Shakya, P. Srivastava, M. Dixit, S.Gambhir, R. K. Shukla & A. Srivastava, An innovative technique for electronic transport model of group-III nitrides, *Scientific Reports* 10, 18706 (2020).
7. PK Saxena, A Srivastava, A Saxena, F Gupta, P Shakya, A Srivastava, et. al., An Innovative Model for Electronic Band Structure Analysis of Doped and Un-Doped ZnO, Journal of Electronic Materials 50 (4), 2417-2424(2021).
8. P. K. Saxena, F. K. Gupta, A. Srivastava, P. Srivastava1 and Anshu Saxena, Ultrafast carrier's dynamics with scattering rate saturation in Ge thinfilmsUltrafast carrier's dynamics with scattering rate saturation in Ge thinfilms TechRxiv · Mar 17, 2022

Thank You

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