



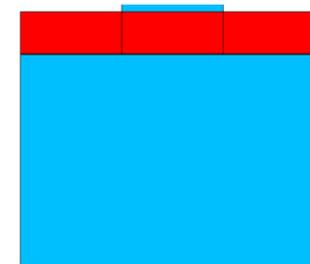
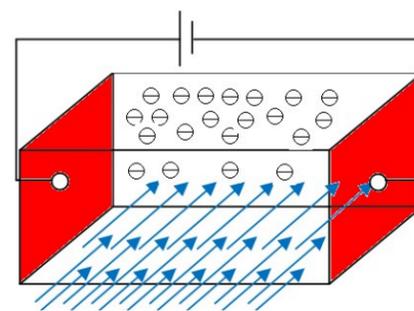
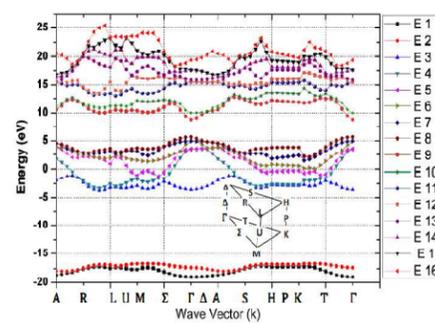
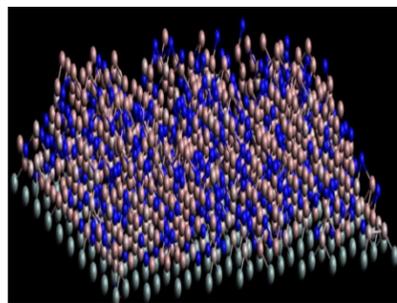
Low- & High-pressure MOCVD Reactors

Epitaxial Growth Solution

Solar Cell



*Technology of Next Level
driven through innovation*



CHALLENGES: SOLAR CELL TECHNOLOGY



- ❑ **III–V Multijunction Solar Cell Integration with Silicon**
- ❑ *Achieving high-efficiency solar cells and at the same time driving down the cell cost*
- ❑ Materials Used : Group III-V Arsenides, Phosphides, and Nitrides, Group IV, IV-VI and II-VI semiconductors
- ❑ III–V compound solar cells: shown performance improvement at ~1% (absolute) increase per year, with a recent record efficiency of 44.7%
- ❑ III–V solar cells on Si substrate through heteroepitaxial integration
- ❑ Among competing photovoltaic technologies, the expensive cost is biggest impediment in their large-scale deployment for terrestrial applications

PERFORMANCE: SOLAR CELL TECHNOLOGY



- Most significant cost III–V solar cells is the cost of substrate.
- Typically, GaAs or Ge substrates used for III–V multijunction solar cell growth,
- Smaller in diameter and significantly more expensive than Si substrate
- Transitioning from a 4" Ge substrate to a 8" Si substrate would reduce 60% cost

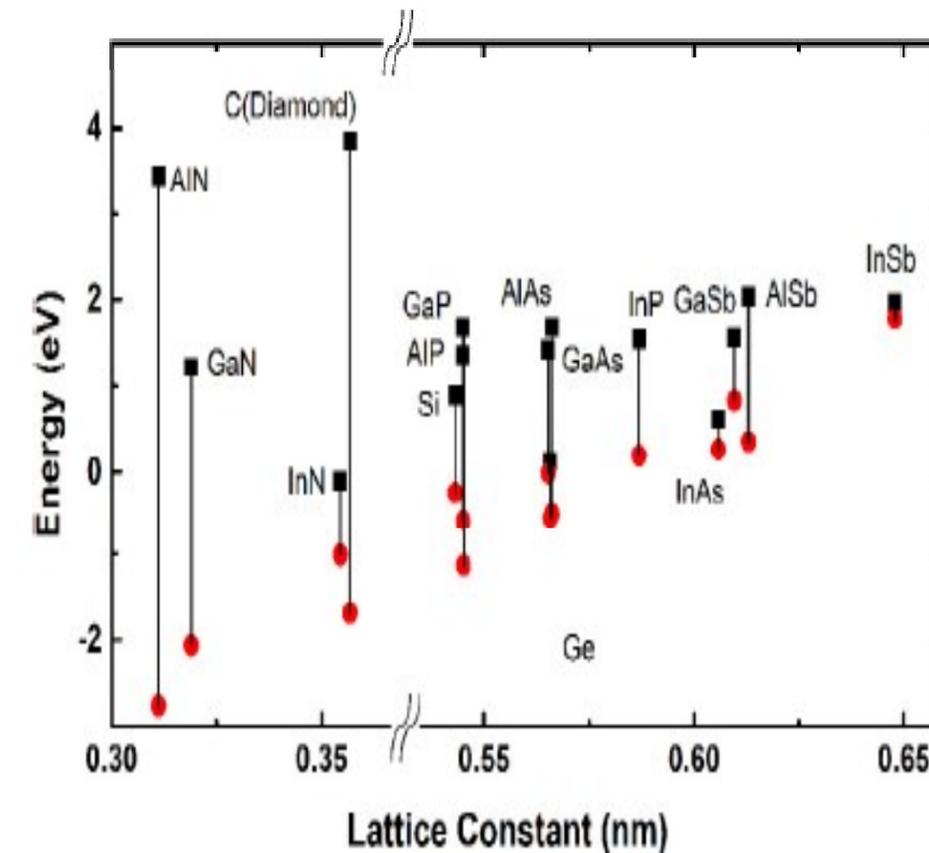
Technology	Efficiency	Room for Improvement
1J Single junction Si	~25%	Saturated
2J InGaP/GaAs based multijunction	32.9% -36.5%	Performance improvement at ~1% increase
3J InGaP/GaAs//Si or III-V Nitrides	~40%	
4J AlGaAs/ GaAs/Si/InGaAs tandem	=44.7%	Reported further room for improvement
Thin strained layers (SLs) and superlattices	~ 35%	To reduce Defects

DESIGN CRITERIA & CHALLENGES



Two key approaches for integrating III–V multijunction solar cells on Si substrate:

- (i) Heteroepitaxial growth: *very promising path with several challenges e.g. lattice mismatch, strain, types of defect generation*
- (ii) Mechanical stacking or wafer bonding: *suffers with wafer bowing or cracking due to large thermal mismatch, free from lattice-mismatch, depends upon Hetroepitaxy growth*



*E.T. Yu, J.O. McCaldin, T.C. McGill, Band offsets in semiconductor heterojunctions, in: E. Henry, T. David (Eds.), Solid State Physics, Academic Press, 1992, pp. 1–146

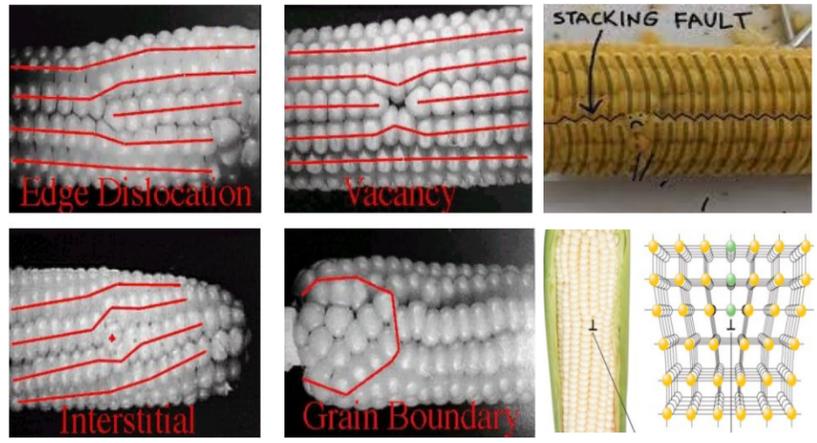


HETEROEPITAXY: CHALLENGES



- ❑ Band gaps Tuning : depends on material thickness, composition, defects etc
- ❑ Efficient absorption from the incident light: thickness of active region
- ❑ High thermal/chemical stability: allow operations in extreme conditions in space
- ❑ 4% lattice-mismatch between GaAs & Si: Epitaxy of GaAs on Si extremely challenging
- ❑ Formation of defects and dislocations
- ❑ Such defects limit solar cell performance

Substrate	Si	Al ₂ O ₃	SiC	Bulk GaN	AlN
Lattice Mismatch (%)	17	16	3.4	-	2.5
Thermal Conductivity	150	35	490	260	319
Resistivity (ohm-cm)	10 ⁴	10 ¹⁴	~10 ¹²	-	>10 ¹⁴



CHALLENGES: GaN/Si EPITAXY



- ❑ *GaN directly on Si or Sapphire* encounters several challenges: large lattice mismatch (16% to 20.4%), thermal expansion coefficient (TEC) mismatch $\sim 53\%$
- ❑ *GaN buffer layer : Avoid formation of cracks and several other technological challenges*
- ❑ *Stacks of $In_xGa_{1-x}N$ layers on GaN buffer layer : To balance compressive and tensile strain*
- ❑ Growth of the GaN buffer layer on the Si substrate : *Still not well understood*
- ❑ Formation of *amorphous SiNx*, deteriorates crystalline quality.
- ❑ Pre-nitridation process of Si substrate greatly influences surface morphology. However, nitridation time and temperature highly influence strain generation
- ❑ 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 or Sapphire substrates

CHALLENGES: GaN/Si EPITAXY



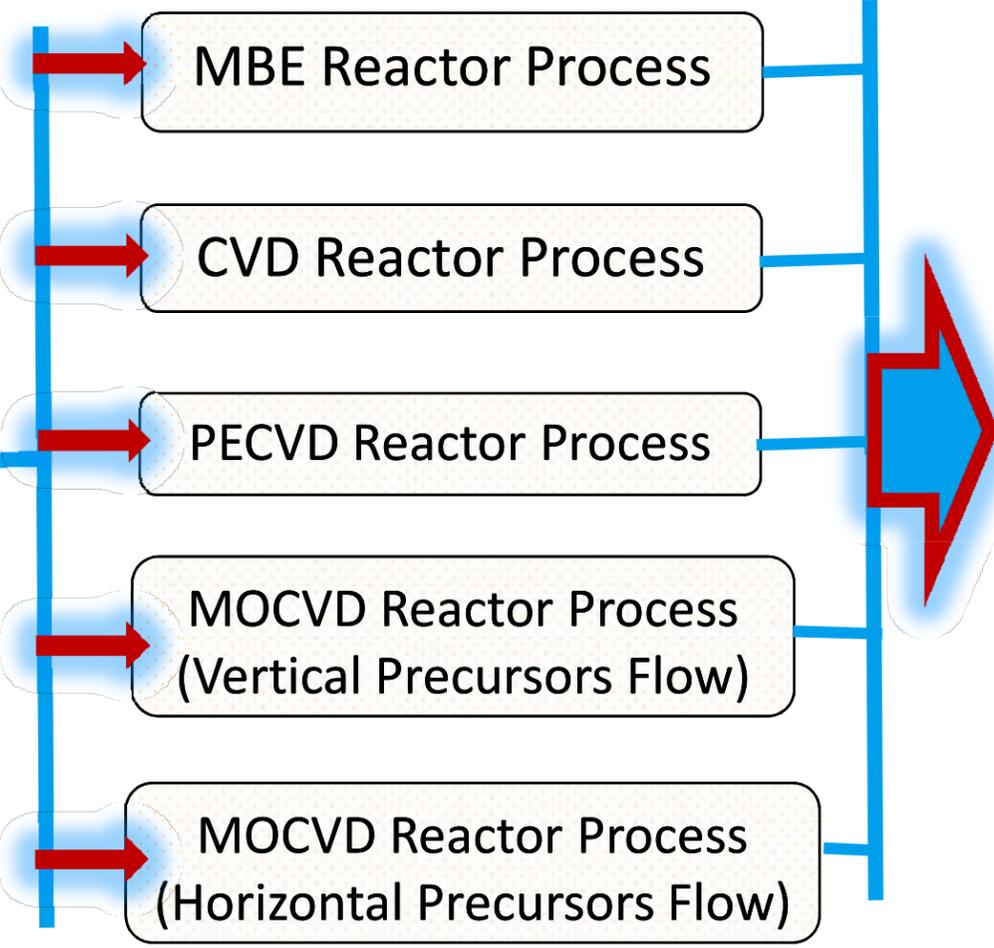
- ❑ GaN-on-Si devices recently attracted much attention *reliable Solar cell* applications due to *cost & large size Si substrates* with possibility of *co-processing in CMOS foundries*
- ❑ Contributor to incident power loss at multiple interfaces due to *parasitic effects*
- ❑ Type of conductivity & formation mechanism of parasitic channel is **controversial**
- ❑ Formation of a p-type conductive channel at the GaN/Si interface,
- ❑ Formation of an n-type electron channel induced by the strong polarization field at the GaN/Si interface.
- ❑ Understanding the behaviors of the parasitic interfaces at multiple junctions: *crucial to reduce the losses*
- ❑ Unsolved problem requires an unambiguous identification of these issues and require lot of investment to do **Hits & Trials**

TNL - EPITAXY PROCESS SOLUTION



Innovative Atomistic Scale Reactor Simulation without use of Continuum models

TNL Framework



- 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.)	<input type="text" value="1.4"/>	
Chamber Pressure	<input type="text" value="10"/>	<input type="text" value="torr"/>
Ceiling Height (cm)	<input type="text" value="2.0"/>	
Chamber Temperature (C)	<input type="text" value="100"/>	
Sticking Coeff.	<input type="text" value="1"/>	

Many More parameters details Require

Precursor Condition

Number of Port

Precursor 1

Flow Rate

Step 1

Precursor Condition

Number of Port

Precursor 1

Flow Rate

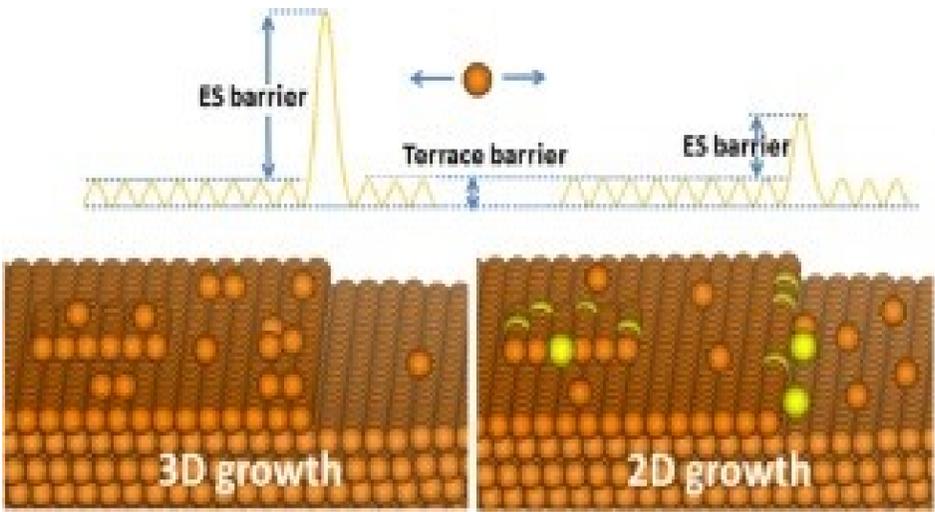
- Select Precursor
- Ga(CH3)3
- (CH3)3CAsH2
- H2
- Al(CH3)3
- NH3
- CH3
- O2



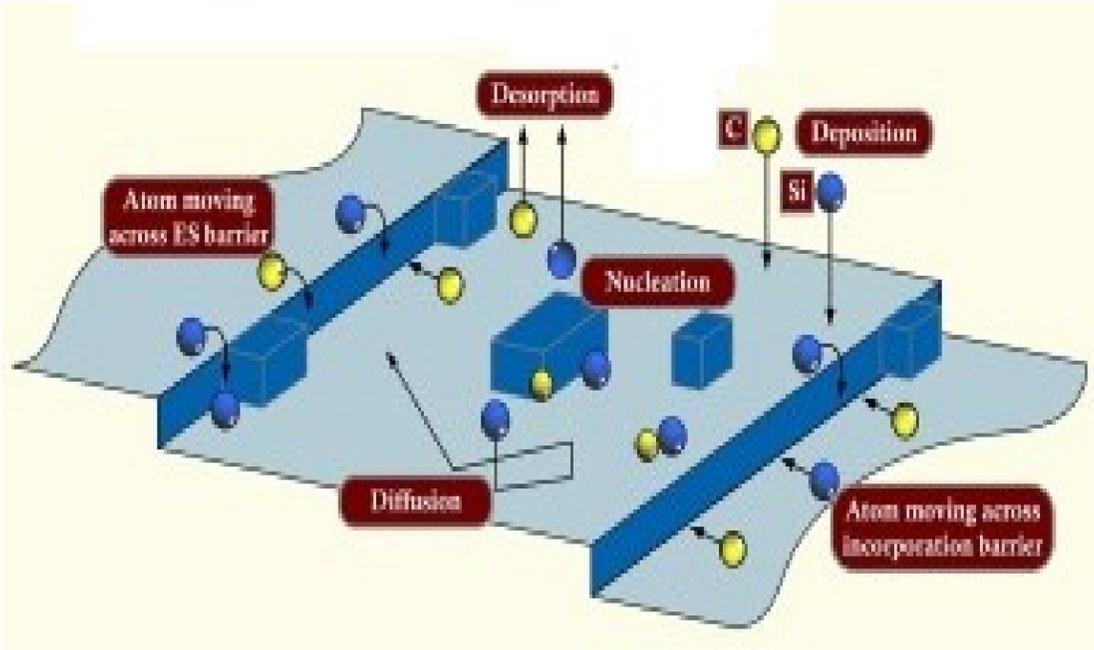
METHODOLOGY: MOCVD PROCESS



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.

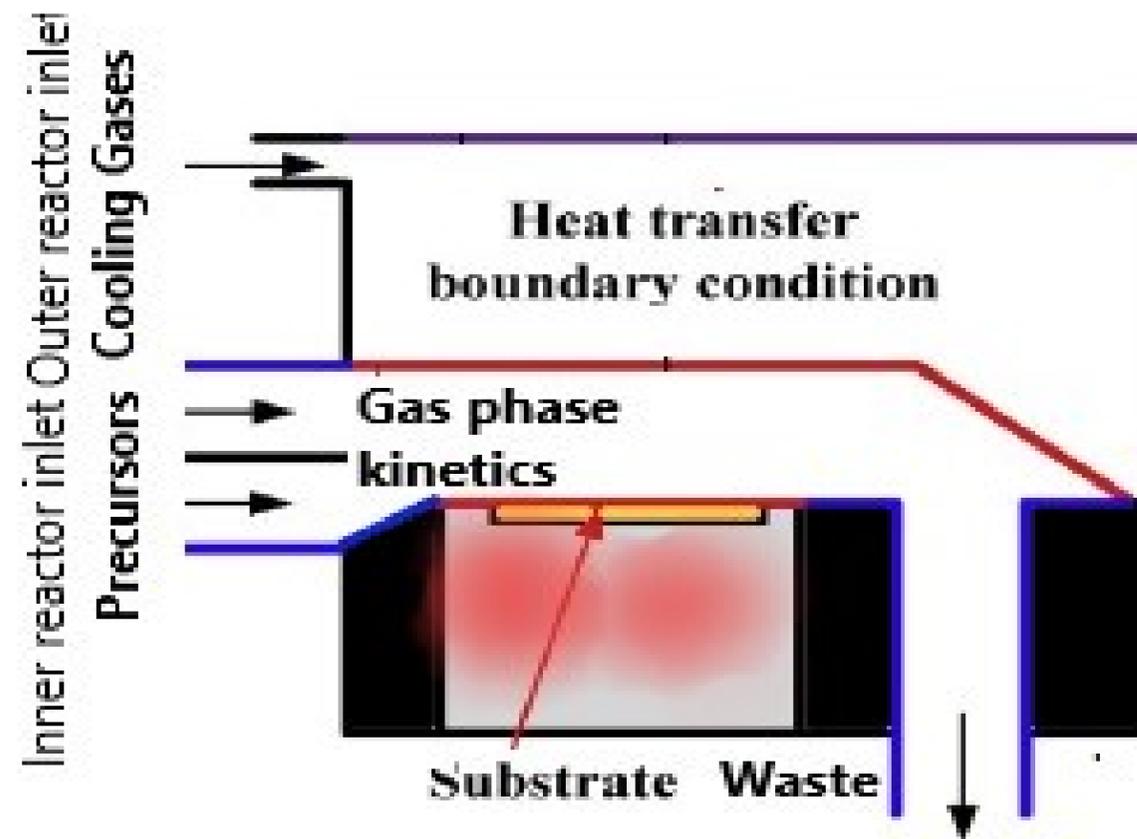


PLANETARY MOCVD PROCESS



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, c_A is the concentration of species A, x is the direction perpendicular to the substrate surface, R is the gas constant, T is the absolute 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 $\Omega_{D,AB}$ 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 $k_s \gg h_g$, the system dictated by mass controlled, low gas transport rate through the boundary layer limits the rapid surface reaction.

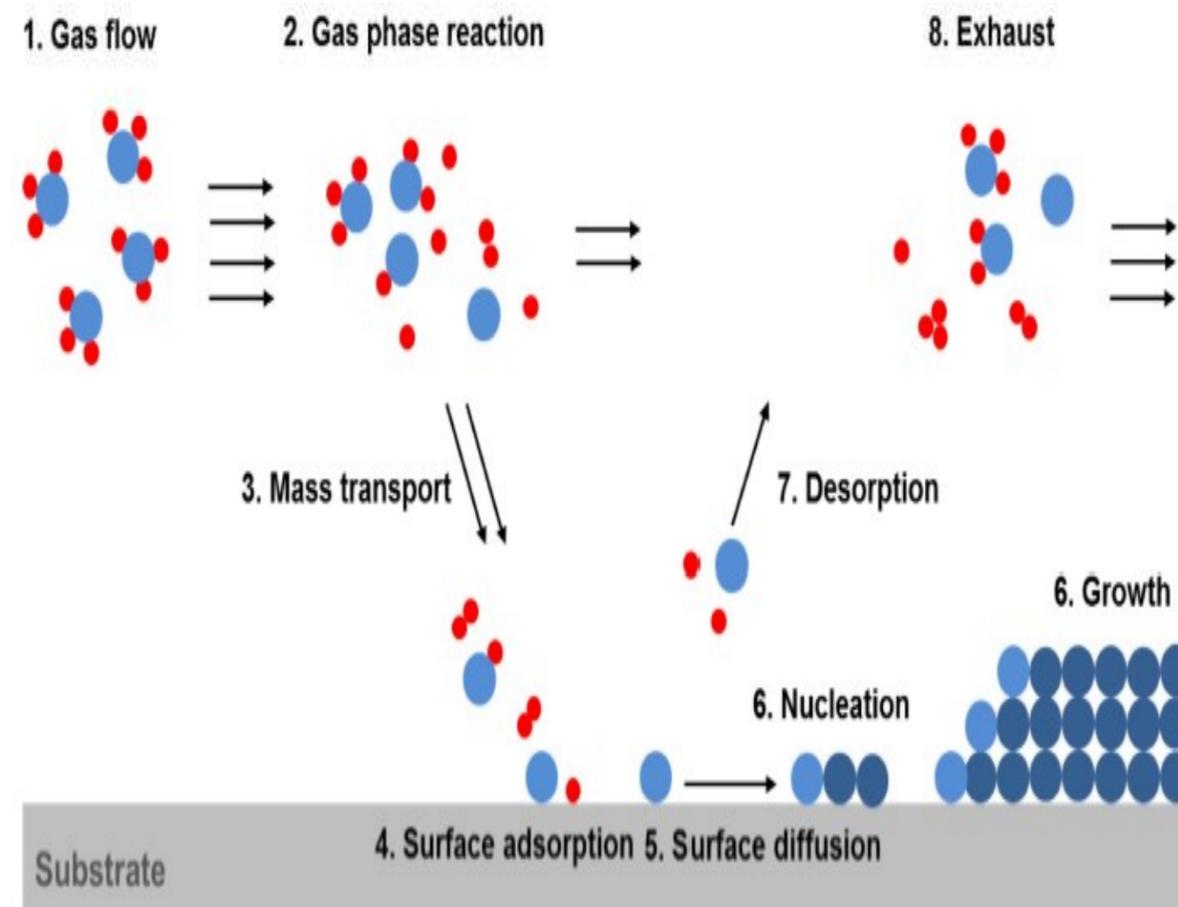
Surface reaction control dominates for $h_g \gg k_s$, the surface reaction is slow even through sufficient reactant gas is available. Additionally, h_g increases with increasing pressure and decreasing temperature and k_s follows the Arrhenius equation.



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.



CHEMICAL KINETICS SOLUTION



- TNL Chemical Kinetics database includes gas- and surface phase chemical reactions
- Users may choose any desired equation or set of equations for the precursors they input based on requirements
- Users have flexibilities to write their own chemical reactions



TNL_Chemical Kinetics

Precursors

H2,SiH4

No.	Name	A	n	E(Cal)
1	G 1 SiH4 --> SiH2 + H2	9.49	1.7	54710
2	G 2 SiH4 + SiH2 --> Si2H6	10.26	1.7	50200
3	G 3 Si2H6 + SiH2 --> HSiSiH3 + ...	14.24	0.4	8900
4	G 4 Si2H6 --> H2 + HSiSiH3	9.96	1.8	54200
5	G 5 HSiSiH3 --> H2SiSiH2	13.40	0.2	5380
6	G 6 HSiSiH3+H2 --> SiH2 + SiH4	13.97	0	4092

No.	Name	A	n	E(Cal)
2	S 2 SiH2 + sigma --> Si+H2	11.76	0.5	0
3	S 3 H2 + 2sigma --> 2H*	11.36	0.5	17250

Output_Window

No.	Gas_Reaction	A	n	E(Cal)
1	G 1 SiH4 --> SiH2 + H2	9.49	1.7	54710
2	G 2 SiH4 + SiH2 --> Si2H6	10.26	1.7	50200
3	G 3 Si2H6 + SiH2 --> HSiSiH3 + SiH4	14.24	0.4	8900
4	G 4 Si2H6 --> H2 + HSiSiH3	9.96	1.8	54200
5	G 5 HSiSiH3 --> H2SiSiH2	13.40	0.2	5380

No.	Surface_Reaction	A	n	E(Cal)
2	S 2 SiH2 + sigma --> Si+H2	11.76	0.5	0
3	S 3 H2 + 2sigma --> 2H*	11.36	0.5	17250

Editor

TNL CHEMICAL DATABASE



Precursors for MN Growth

(M = Ga, Al, In)

TMM, DMM, NH₃, AsH₃, PH₃, TBP etc.

Dopants

Cp₂ Mg, SiH₄, DEZ, DETe, CBrCl₃ etc.

Carrier Gases: MN Growth

N₂, H₂, Ar etc.

Here,

TBP- tertbutylphosphine

DEZ- DiethylZinc

DETe- DiethylTelluride

CBrCl₃- Bromotrichloromethane



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

Reaction rates in forward and reverse directions

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



TMG, NH₃ & N₂/H₂/ARGON



Gas-phase Mechanisms Reactions

		$k = AT^n e^{-E_a/RT}$					A	n	E_a
G1	TMG	=	DMG	+	CH ₃		1.00×10^{47}	-9.18	76,996
G2	DMG	=	MMG	+	CH ₃		7.67×10^{43}	-9.8	34,017
G3	MMG	=	Ga	+	CH ₃		1.68×10^{30}	-5.07	84,030
G4	TMG	+	NH ₃	→	TMG:NH ₃		2.28×10^{34}	-8.31	3115
G5	TMG	+	NH ₃	→	DMG:NH ₂	+	CH ₄	2	19,969
G6	DMG	+	NH ₃	→	DMG:NH ₃		4.08×10^{31}	-7.03	3234
G7	DMG	+	NH ₃	→	MMG:NH ₂	+	CH ₄	1.56	20,744
G8	MMG	+	NH ₃	→	MMG:NH ₃		7.95×10^{24}	-5.21	2094
G9	MMG	+	NH ₃	→	GaNH ₂	+	CH ₄	1.3	17,722
G10	NH ₃	+	CH ₃	→	NH ₂	+	CH ₄	2.51	9859
G11	CH ₃	+	H ₂	→	CH ₄	+	H	0	12,518
G12	TMG	+	H	→	DMG	+	CH ₄	0	10,036
G13	DMG	+	H	→	MMG	+	CH ₄	0	10,036
G14	TMG:NH ₃	→	MMG	+	2CH ₃	+	NH ₃	-8.24	77,791
G15	CH ₃	+	H	+	M	→	CH ₄ + NH ₃	-1	0
G16	2CH ₃	=	C ₂ H ₆				2.00×10^{13}	0	0
G17	2H	+	M	=	H ₂	+	M	0	0



TMG, NH₃ & N₂/H₂/ARGON



Surface phase Reactions: PATH 1

Path 1, $k = AT^n e^{-E_a/RT}$					A	n	E _a	
1	MMG	+	N(S)	→	MMG(S)	1.16×10^5	2.98	0
2	MMG(S)	→	MMG	+	N(S)	1.12×10^{14}	0.55	107,673
3	NH ₃	+	MMG(S)	→	COMPM1(S)	3.35×10^7	3.33	0
4	COMPM1(S)	→	NH ₃	+	MMG(S)	5.70×10^{13}	-0.16	8146
5	MMG	+	COMPM1(S)	→	CH ₄ + COMPM2(S)	1.23×10^{10}	3.22	23,446
6	NH ₃	+	COMPM2(S)	→	COMPM3(S)	3.35×10^7	3.33	0
7	COMPM3(S)	→	NH ₃	+	COMPM2(S)	5.70×10^{13}	-0.161	8146
8	MMG	+	COMPM3(S)	→	CH ₄ + COMPM4(S)	1.23×10^{10}	3.22	23,446
9	NH ₃	+	COMPM4(S)	→	COMPM5(S)	3.35×10^7	3.33	0
10	COMPM5(S)	→	NH ₃	+	COMPM4(S)	5.70×10^{13}	-0.161	8146
11	COMPM5(S)	→	CH ₄	+	RINGM1(S)	1.23×10^7	3.22	23,446
12	Ga(S)	+	RINGM1(S)	→	RINGM2(S) + N(S)	3.35×10^7	3.33	0
13	RINGM2(S)	→	3H ₂	+	3GaN(B) + Ga(S)	3.68×10^9	2.05	59,610



TMG, NH₃ & N₂/H₂/ARGON



Surface phase Reactions: PATH 2

	Path 2, $k = AT^n e^{-E_a/RT}$				A	n	E _a	
14	CH ₃	+	Ga(S)	→	MMG(S)	1.76 × 10 ⁹	1.39	0
15	MMG(S)	→	CH ₃	+	Ga(S)	4.54 × 10 ¹³	0.0346	79,480
16	NH ₂	+	Ga(S)	→	NH ₂ (S)	3.17 × 10 ⁸	1.83	0
17	GaNH ₂	+	N(S)	→	GaNH ₂ (s)	2.27 × 10 ⁶	2.247	0
18	GaNH ₂ (S)	→	GaNH ₂	+	N(S)	4.83 × 10 ¹³	0.614	83,881
19	COMPMM1(S)	→	CH ₄	+	GaNH ₂ (S)	1.49 × 10 ¹¹	0.609	25,950
20	MMG	+	GaNH ₂ (S)	→	COMPMM1(S)	1.16 × 10 ⁵	2.98	0
21	NH ₃	+	COMPMM1(S)	→	COMPMM2(S)	3.35 × 10 ⁷	3.33	0
22	COMPMM2(S)	→	CH ₄	+	COMPMM3(S)	1.49 × 10 ¹¹	0.609	25,950
23	MMG	+	COMPMM3(S)	→	COMPMM4(S)	1.16 × 10 ⁵	2.98	0
24	NH ₃	+	COMPMM4(S)	→	COMPMM5(S)	3.35 × 10 ⁷	3.33	0
25	COMPMM5(S)	→	CH ₄	+	RINGM1(S)	1.49 × 10 ¹¹	0.609	25,950
26	NH ₂ (S)	→	NH ₂	+	Ga(S)	1.45 × 10 ¹⁴	0.09	59,786
27	COMPMM1(S)	→	MMG	+	GaNH ₂ (S)	1.00 × 10 ¹⁴	0.55	42,819
28	COMPMM2(S)	→	NH ₃	+	COMPMM1(S)	5.70 × 10 ¹³	-0.1	8146
29	COMPMM4(S)	→	MMG	+	COMPMM3(S)	1.00 × 10 ¹⁴	0.55	42,819
30	COMPMM5(S)	→	NH ₃	+	COMPMM4(S)	5.70 × 10 ¹³	-0.1	8146
31	Ga	+	N(S)	→	Ga(S)	1.00 × 10 ¹¹	1.5	0
32	Ga(S)	+	NH ₂ (S)	→	GaNH ₂ + Ga(S)	1.00 × 10 ²⁵	0	0
33	Ga(S)	→	Ga	+	N(S)	1.00 × 10 ¹³	0	45,168
34	6CH ₃	+	RINGM2(S)	→	COM1(S)	7.55 × 10 ⁷	2.31	0
35	COM1(S)	→	6CH ₃	+	RINGM2(S)	1.00 × 10 ¹³	0.71	45,506
36	COM1(S)	→	6CH ₄	+	3GaN(B) + Ga(S)	4.00 × 10 ¹²	0	49,675



TMG, NH₃ & N₂/H₂/ARGON



Surface phase Reactions: PATH 3

	Path 3, $k = AT^n e^{-E_a/RT}$					A	n	E _a
37	TMG	+	N(S)	→	TMG(S)	1.16×10^5	2.98	0
38	NH ₃	+	TMG(S)	→	TCOM1(S)	3.35×10^7	3.33	0
39	TCOM1(S)	→	CH ₄	+	TCOM2(S)	1.49×10^{11}	0.609	32,785
40	Ga(S)	+	TCOM2(S)	→	TCOM3(S) + N(S)	3.35×10^7	3.33	0
41	TCOM3(S)	→	2CH ₄	+	GaN(B) + Ga(S)	1.49×10^{11}	0.609	49,675
42	TMG(S)	→	TMG	+	N(S)	1.12×10^{14}	0.55	49,675
43	TCOM1(S)	→	NH ₃	+	TMG(S)	5.70×10^{13}	-0.161	11,922
44	TMG:NH ₃	+	N(S)	→	TCOM1(S)	1.16×10^5	2.98	0
45	TCOM1(S)	→	TMG:NH ₃	+	N(S)	1.12×10^{14}	0.55	49,675
46	TCOM1(S)	→	2CH ₃	+	MMG(S) + NH ₃ + N(S)	1.12×10^{14}	0.55	10,7673
47	MMGNH ₃	+	N(S)	→	COMPM1(S)	1.16×10^5	2.98	0
48	COMPM1(S)	→	MMG:NH ₃	+	N(S)	1.12×10^{14}	0.55	107,673
49	MMG:NH ₃	+	COMPM1(S)	→	CH ₄ + COMPM3(S)	1.23×10^{10}	3.22	23,446
50	MMG:NH ₃	+	COMPM3(S)	→	CH ₄ + COMPM5(S)	1.23×10^{10}	3.22	23,446
51	MMG:NH ₃	+	GaNH ₂ (S)	→	COMPMM2(S)	1.16×10^5	2.98	0
52	MMG:NH ₃	+	COMPMM3(S)	→	COMPMM5(S)	1.16×10^5	2.98	0



METHODOLOGY: 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

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

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 \bar{h} 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	TMAI & NH ₃	TMAI & 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



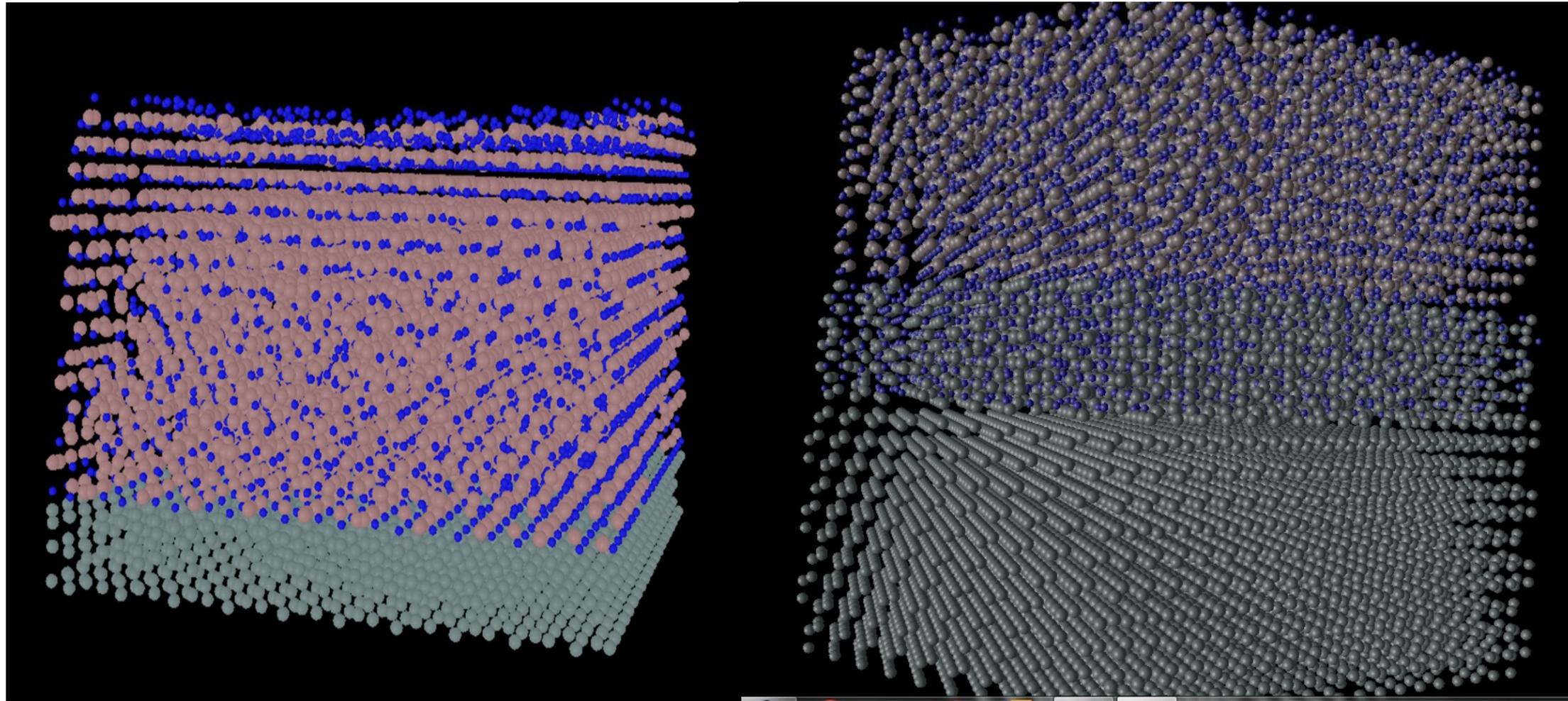
Gas Phase Equations

$\text{Al}(\text{CH}_3)_3 = \text{AlCH}_3 + 2\text{CH}_3,$	$A=3.5 \cdot 10^{15},$	$n=0,$	$E_a= 66500$
$\text{Al}(\text{CH}_3)_3 + \text{NH}_3 = \text{Al}(\text{CH}_3)_3:\text{NH}_3,$	$A=3.0 \cdot 10^{12}$	$n=0$	$E_a= 0.0$
$\text{Al}(\text{CH}_3)_3:\text{NH}_3 = \text{Al}(\text{CH}_3)_3 + \text{NH}_3,$	$A=5.0 \cdot 10^{10}$	$n=0$	$E_a= 22000$
$\text{Al}(\text{CH}_3)_3:\text{NH}_3 = (\text{CH}_3)_2\text{Al}:\text{NH}_2 + \text{CH}_4,$	$A=2.0 \cdot 10^{12}$	$n=0$	$E_a= 27000$
$\text{Al}(\text{CH}_3)_3:\text{NH}_3 + \text{NH}_3 = (\text{CH}_3)_2\text{Al}:\text{NH}_2 + \text{CH}_4 + \text{NH}_3,$	$A=2.0 \cdot 10^{12}$	$n=0$	$E_a= 13000$
$2(\text{CH}_3)_2\text{Al}:\text{NH}_2 = ((\text{CH}_3)_2\text{Al}:\text{NH}_2)_2,$	$A=4.0 \cdot 10^{11}$	$n=0$	$E_a= 0.0$

##Gas to Surface Phase Equations

$\text{Al}(\text{CH}_3)_3 + \text{space} = \text{Al}(\text{S}) + 3\text{CH}_3,$	coll 1.0
$\text{Al}(\text{CH}_3)_3:\text{NH}_3 + \text{space} = \text{Al}(\text{S}) + 3\text{CH}_3 + \text{NH}_3,$	coll 1.0
$\text{AlCH}_3 + \text{space} = \text{Al}(\text{S}) + \text{CH}_3,$	coll 1.0
$(\text{CH}_3)_2\text{Al}:\text{NH}_2 + \text{space} = \text{AlN}(\text{S}) + 2\text{CH}_4,$	coll 1.0
$((\text{CH}_3)_2\text{Al}:\text{NH}_2)_2 + \text{space} = 2\text{AlN}(\text{S}) + 4\text{CH}_4,$	coll 1.0

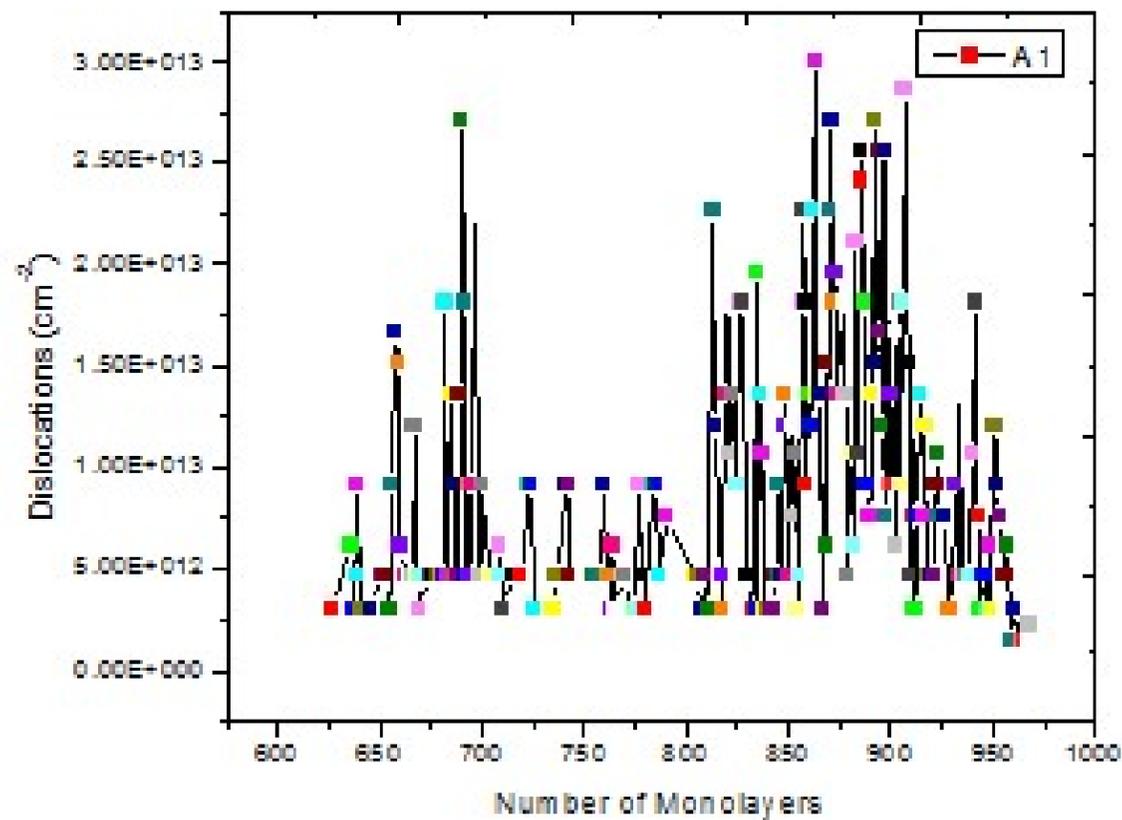
OUTPUT



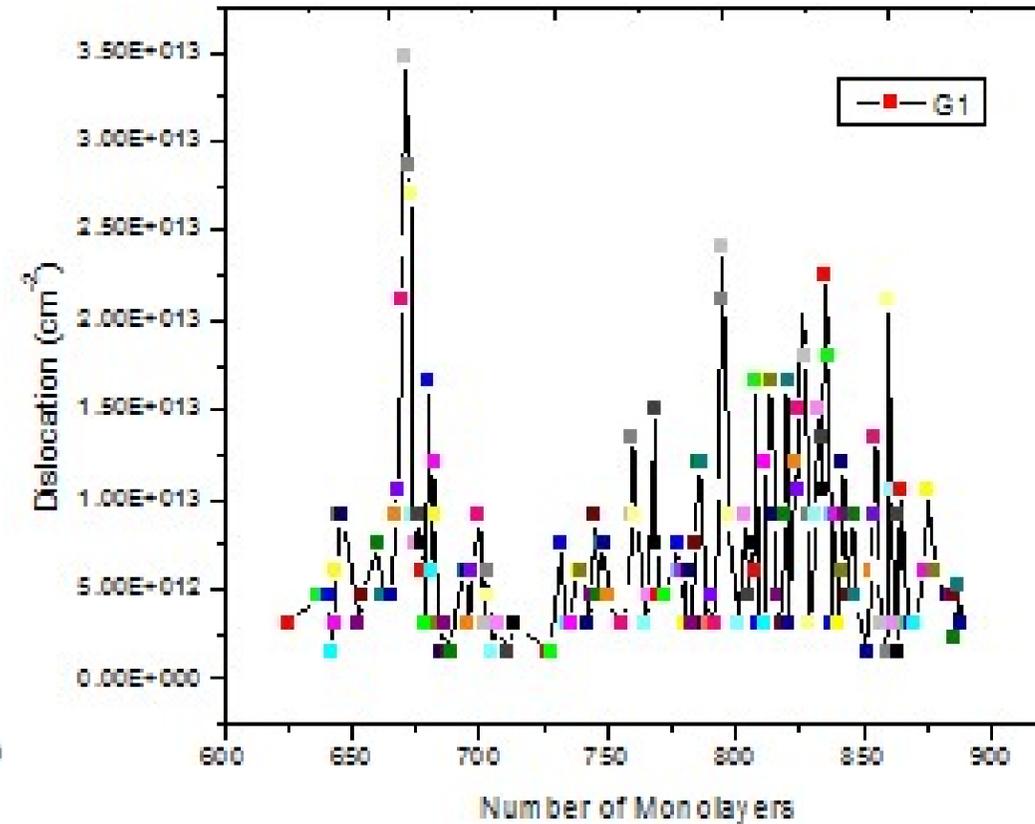
Without Nitridation

Pre-Nitridation for 30 s

DISLOCATIONS PER MONOLAYER

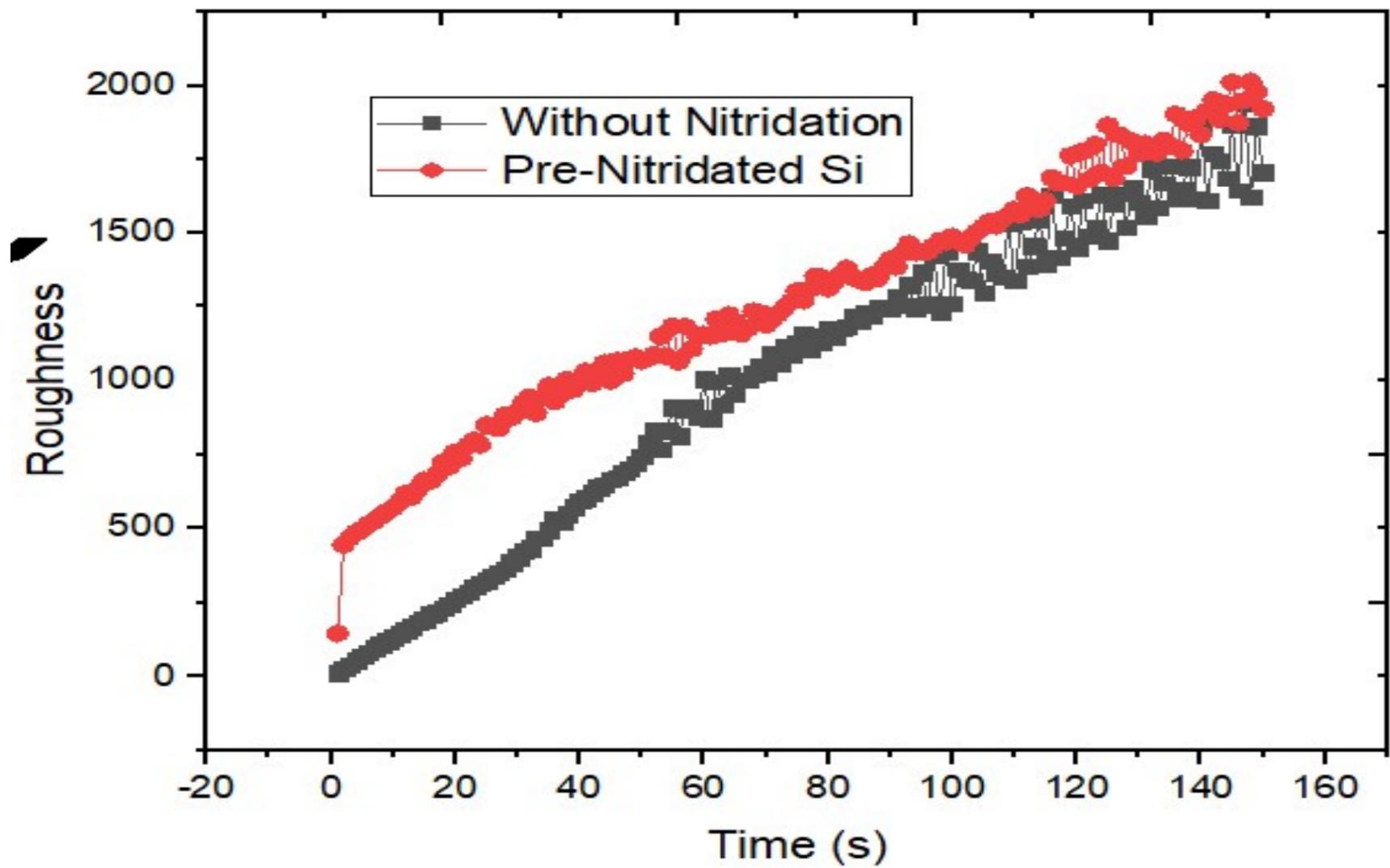


Without Nitridation



Pre-Nitridation for 30 s

SURFACE ROUGHNESS



OTHER OUTPUT

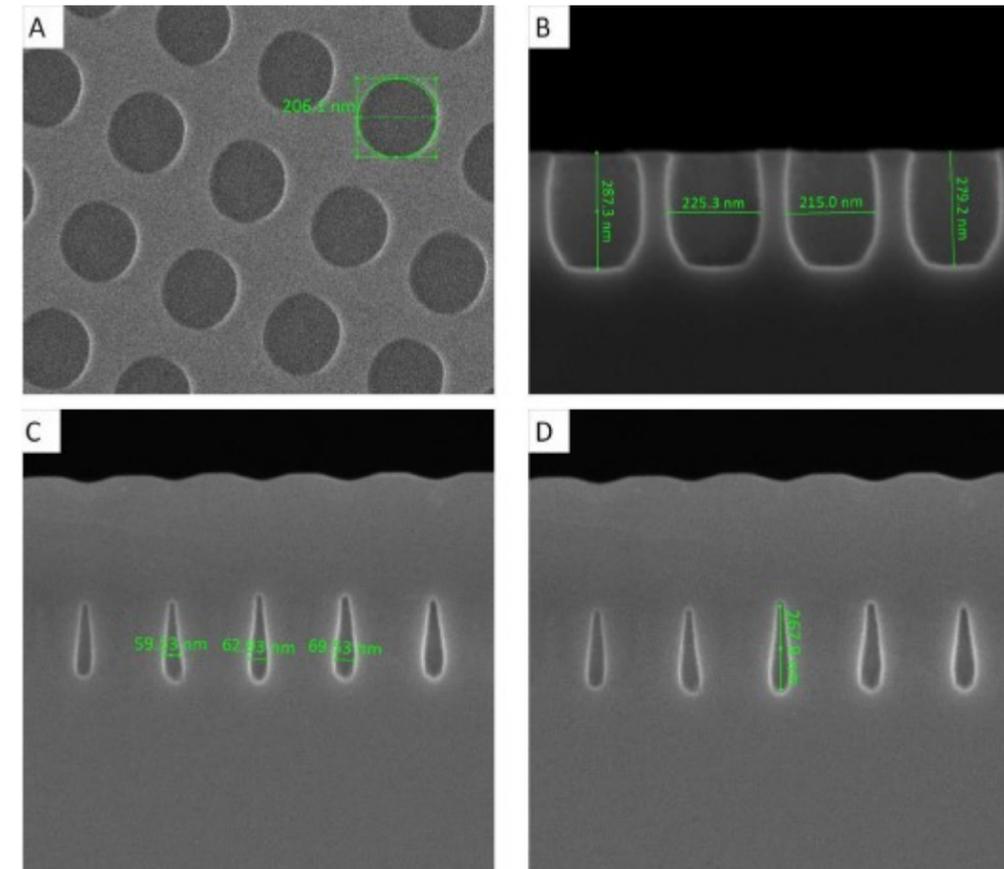
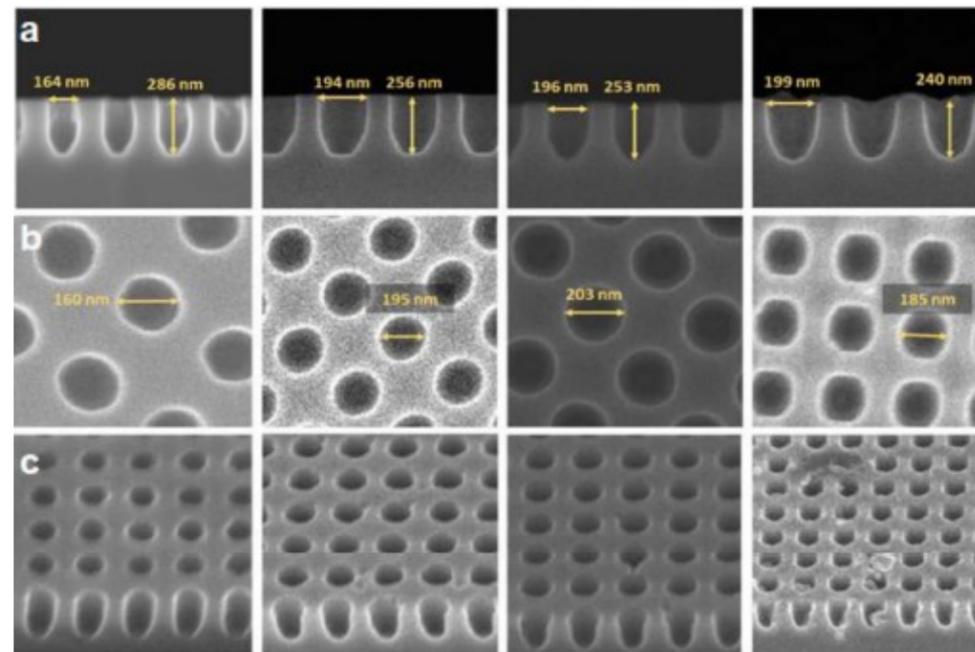
Parameters	Si/AlN	Pre-Nitridated Si /AlN
Substrate Thickness (μm)	0.3258	0.3258
Si ₃ N ₄ Thickness (nm)	-	3.7817
Total Deposited Atoms (AlN)	5046178	5233815
Vacancies (cm^{-3})	36069	13393
Total Dislocation Density (cm^{-3})	2503	1612
Al Atoms	$\approx 50\%$	$\approx 50\%$
N Atoms	$\approx 50\%$	$\approx 50\%$
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

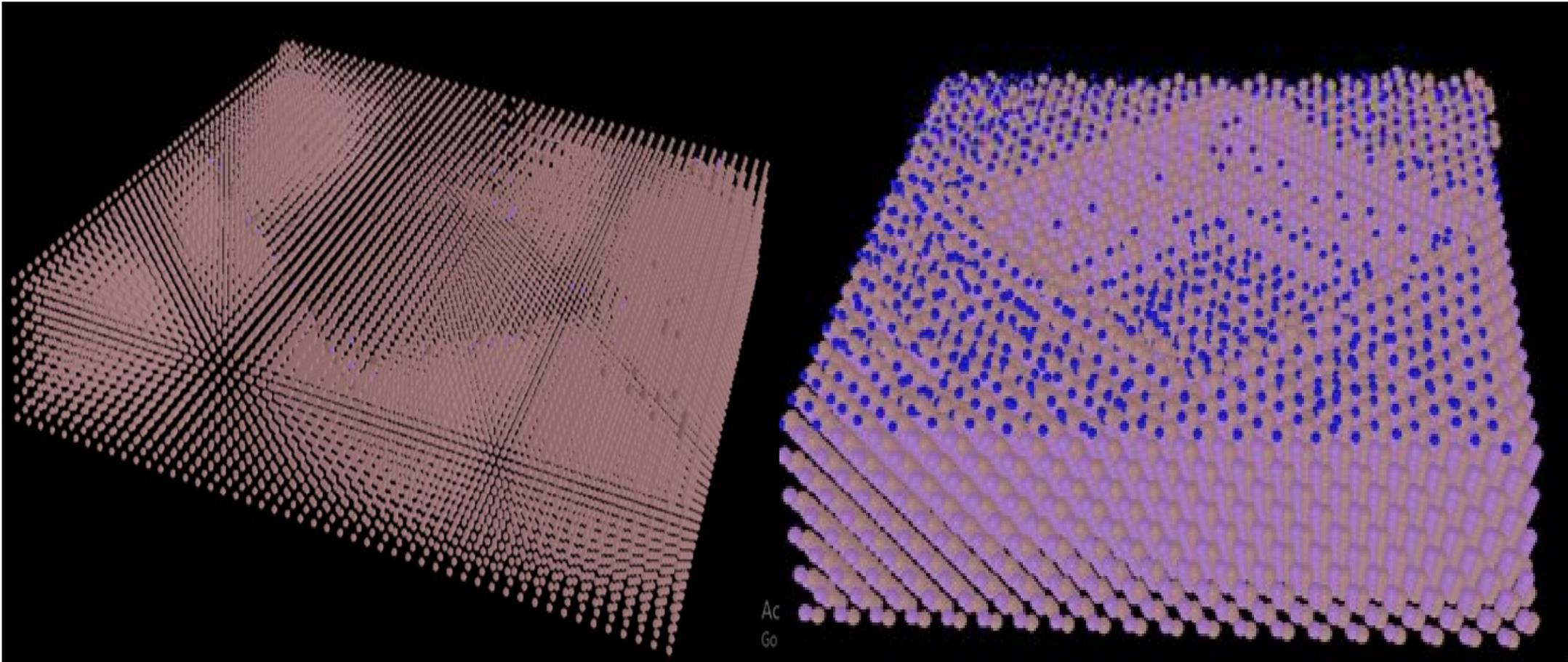


Information

Strictly Private and Confidential



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



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3. Praveen Saxena, R. Trigunayat, Anchal Srivastava, Pankaj Srivastava, Md. Zain, R.K. Shukla, Nishant Kumar, Shivendra Tripathi, FULL ELECTRONIC BAND STURCTURE ANALYSIS OF Cd DOPED ZnO THIN FILMS DEPOSITED BY SOL-GEL SPIN COATING METHOD , II-VI US Workshop Proceedings, 2019.
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Thank You
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