

Role of High Crystalline Quality Material Growth in Improving Semiconductor Device Characteristics

Technology of Next Level
driven through innovation

Atomistic TNL TCAD Solution

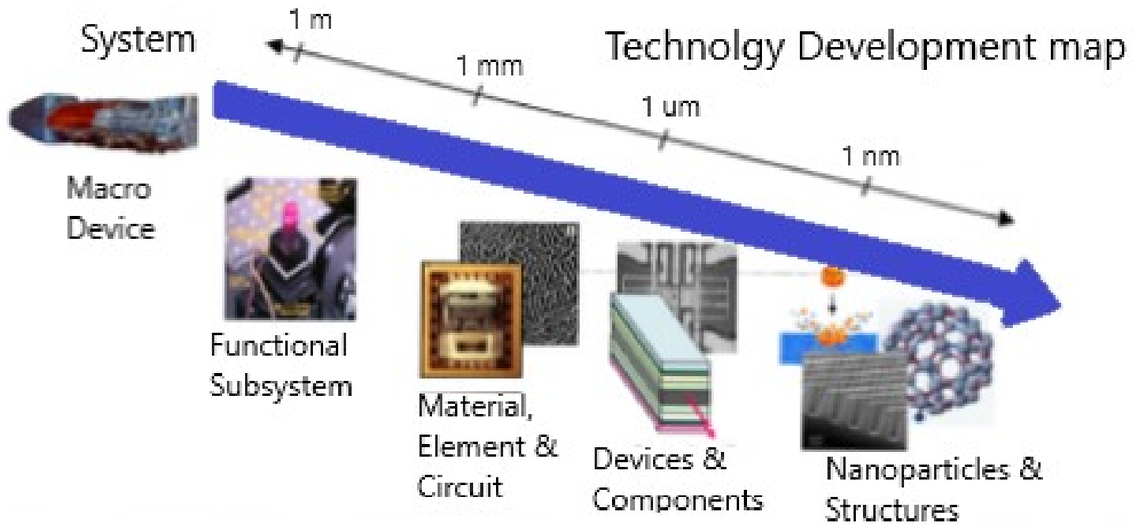
(Atom to Device Simulation)

Angstrom Era : An Innovative Approach

TNL Framework

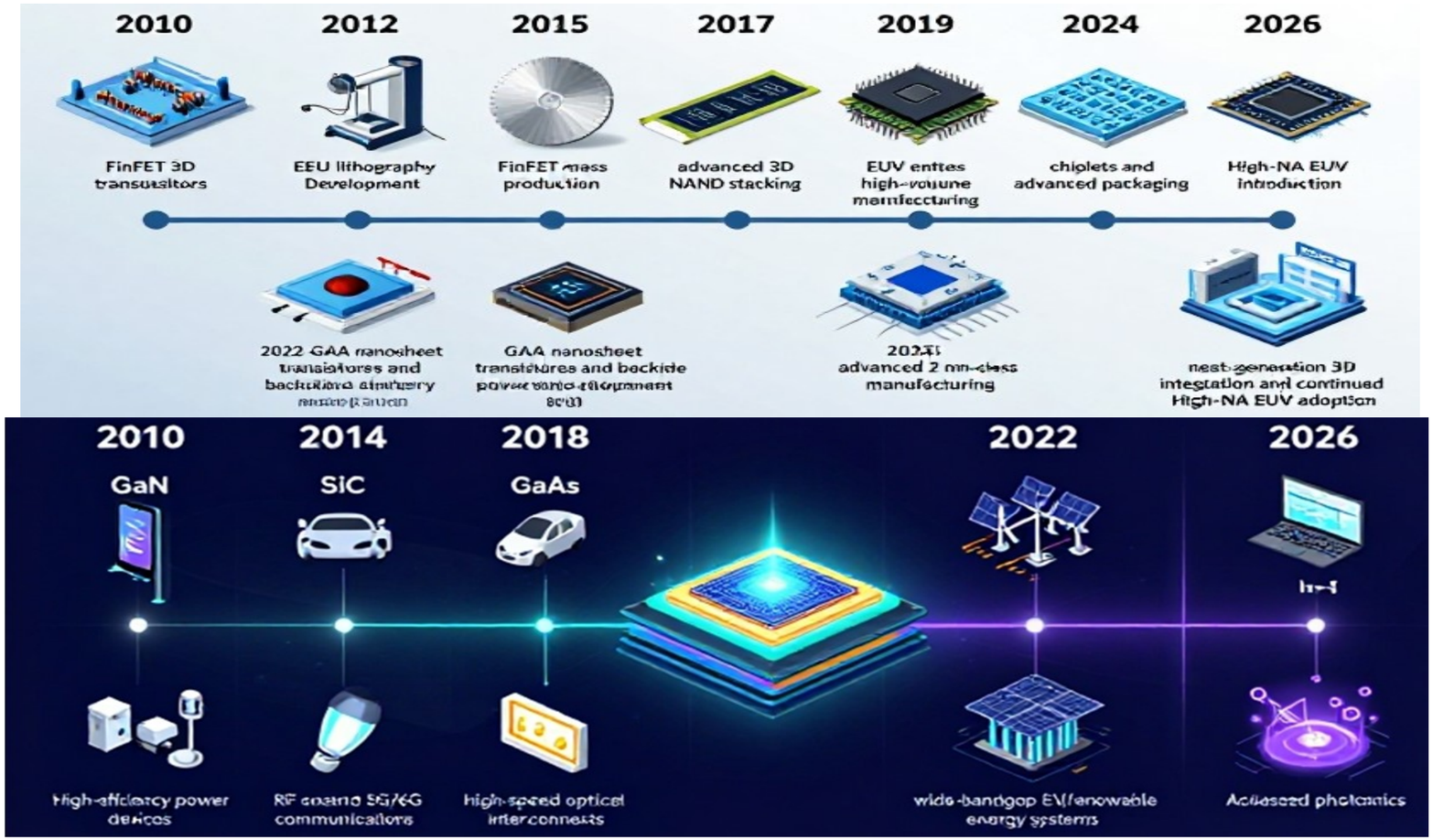
Development: Nature Vs. Technology





- Technology R & D to Production: Require development ***time cycle*** with the investment of ***Huge money***
- Lot of ***technological challenges*** need to be addressed before production starts

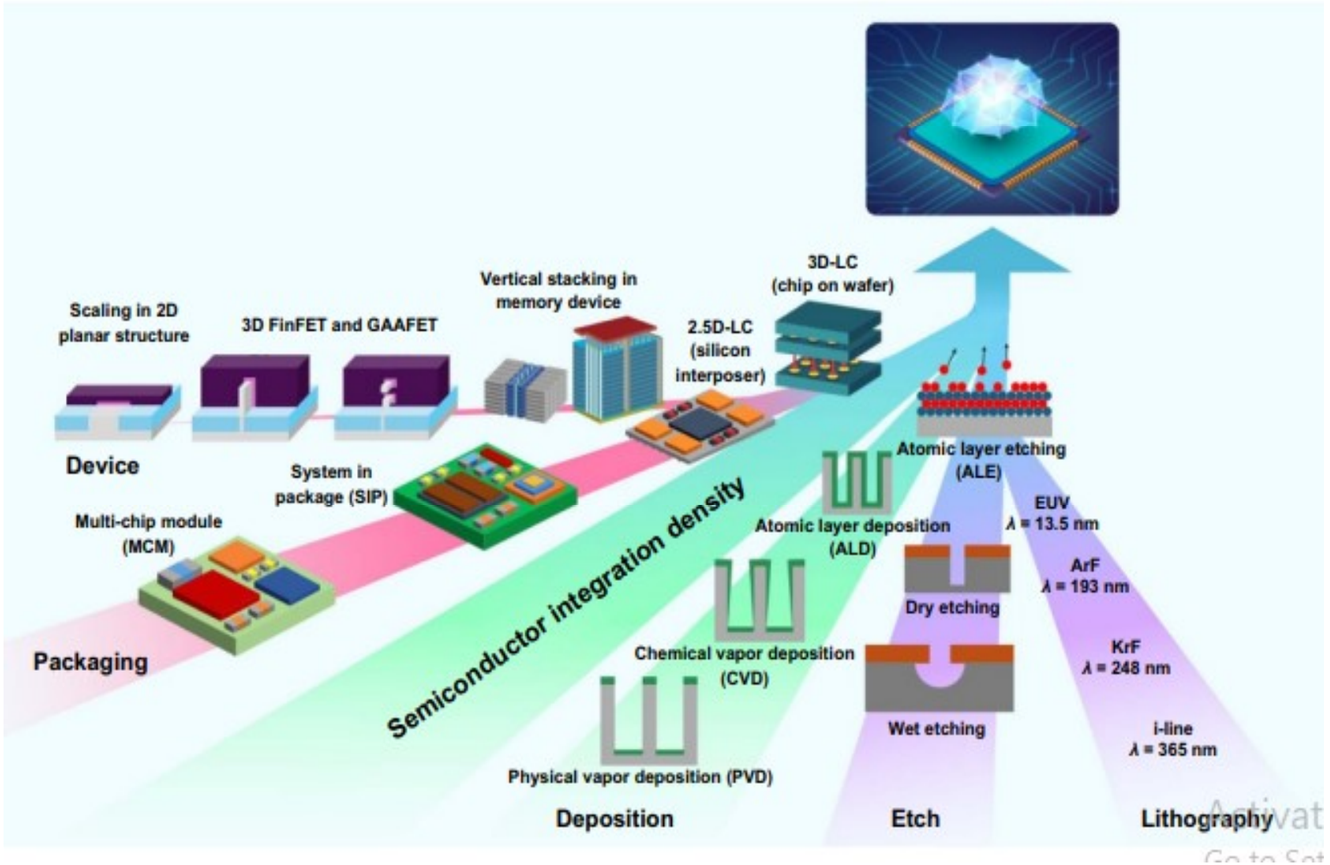
Major Semiconductor Technologies



Transistor: manufacturing process precision

Highlights how increasing integration demands have driven the shift from 2D planar devices to advanced 3D architectures such as FinFET/GAAFET, vertically stacked memory, and 2.5D/3D packaging.

2.5 or 3D integration uses a standard silicon interposer with high-density Through-Silicon Vias (TSVs) for complexity & cost reduction to match CTE.



Scaling from planar to 3D

- Industry relied on *planar/geometrical* scaling to miniaturize transistors and interconnects, delivering improved performance, reduced power consumption, and increased circuit density (Moore's law), ONLY upto **10**-*nm technology node*.
- Below 10 nm-scale gate dimensions, quantum mechanical effects e.g. tunneling, leakage currents, and short-channel distortions significantly degrade optimal performance, *conventional 2D scaling failed*.
- Adopting vertical structuring, e.g. FinFETs, gate-all-around (GAA) nanosheets and CFET architectures : enabled enhanced current control and reduced leakage, but ONLY upto *4-nm technology node*
- In advanced packaging (heterogeneous integration), a growing demand to increase the input/output (I/O) density, bump pitch size is expected to be reduced to below 1 µm, enabling a bump density of $10^6/mm^2$ and achieving a power consumption of less than 0.01 pJ/bit
- Shift from conventional “shrinking” paradigm toward a new era of “restructuring and reprocessing requires atomistic-scale precision in deposition, etching, and patterning

Major Players

- *TECHNEXT LAB (TNL)*: (2015) provides family of angstrom-scale precision simulation software, major emphasis on reactor based epitaxy to improve device performance.

- Applied Angstrom Technology (AAT): (2023) equipment company, builds AI-native atomic layer etch (ALE) platforms for sub-3nm logic, 3D memory, and Si photonics,
- ASM (Advanced Semiconductor Materials): industry-leading atomic layer deposition (ALD) and epitaxy solutions for 3D scaling down to the Ångström scale
- Shenzhen Angstrom Excellence Technology Co. Ltd: (2020), manufactures semiconductor front-end optical and X-ray metrology and inspection equipment
- Angstrom Global Inc.: (2005) AI-powered metrology, intelligent robotics, automated facility solutions, and engineering tools for atomic-scale measurement
- Angstrom Advanced Inc.: atomic force microscopes (AFMs), X-ray diffraction equipment, and scanning electron microscopes

3D Scaling Challenges (Transistor)

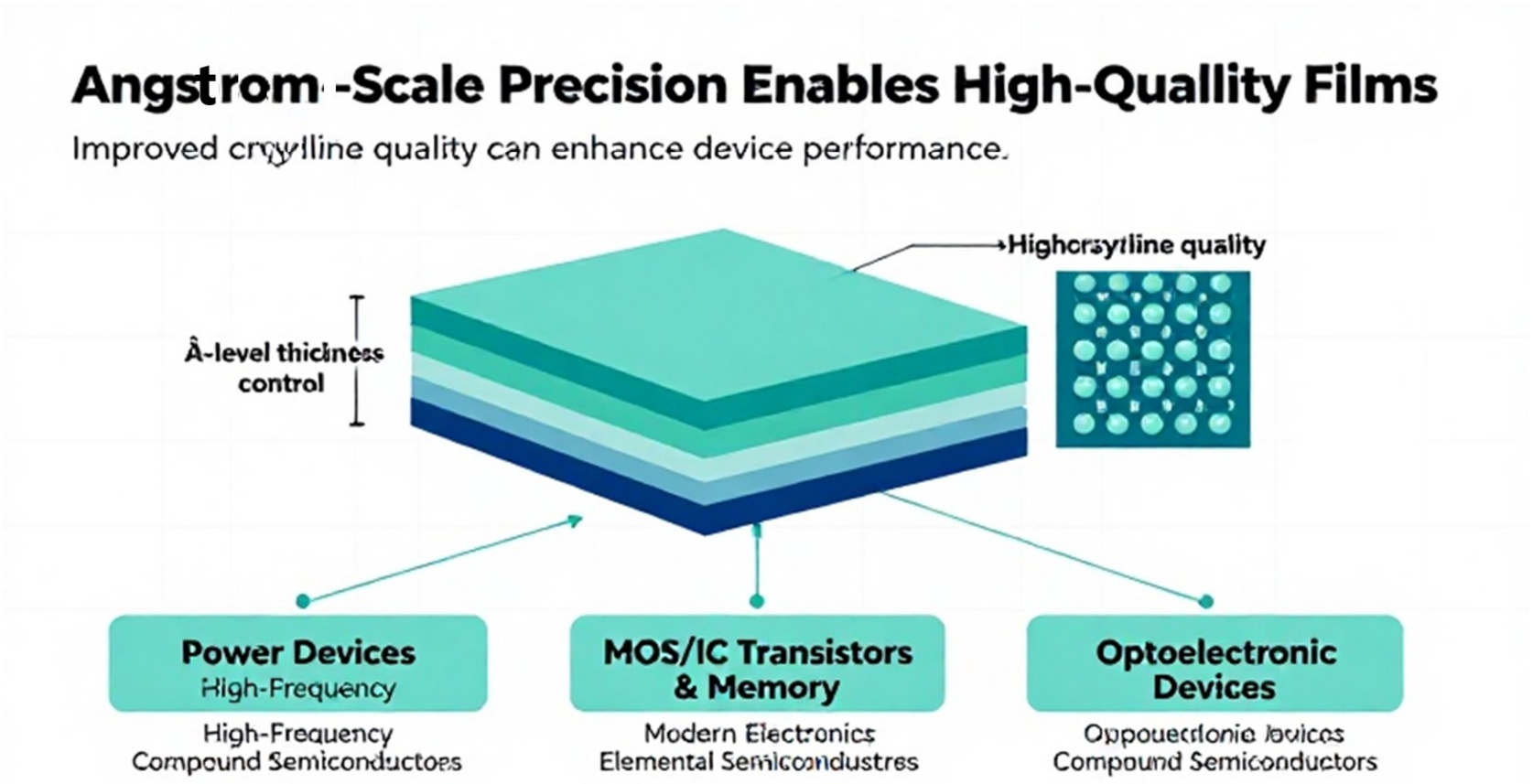
- As device architectures advance, manufacturing must achieve enhanced uniformity and selectivity in constrained 3D configurations.
- Combination of CVD and RIE remain essential for structure definition, both face *reproducibility issue with* uniform, damage-free processing within high-aspect-ratio features.
- Control of precursor transport disparities in CVD, causing film heterogeneity, and RIE experiences aspect ratio-dependent etching and sidewall degradation that impede precise profile control.
- Extreme-ultraviolet (EUV) optical lithography enables sub-10-nm patterns, but faces challenges including *high equipment costs*, *limited capacity, and defect management*.
- Edge placement error, photoresist sensitivity, and line edge roughness collectively demonstrate fundamental challenges of top-down patterning

Challenges (Power & Optoelectronics):

III-V (N, As, P, Sb), III-VI (GaO_2, GeO_2) & 2D (MoS_2, WeS_2) Materials Growth

- ❑ Role of CVD and its variants reactor geometry and its influence on chemistry
- ❑ Reaction mechanism dependency on different energy barriers at surface
- ❑ Surface diffusion predictions along with desorption processes
- ❑ Predictions of growth mechanisms and mode, morphology, doping & parasitics
- ❑ Formation of defects and differentiation among them
- ❑ Strain relaxation on a layer-by-layer basis.
- ❑ Impact of chamber pressures
- ❑ Undesired atomic diffusion from one material layer to other material layer
- ❑ Several other unseen issues
- ❑ *Reproducibility of Experiments*
- ❑ *Huge investment require to optimize a process*

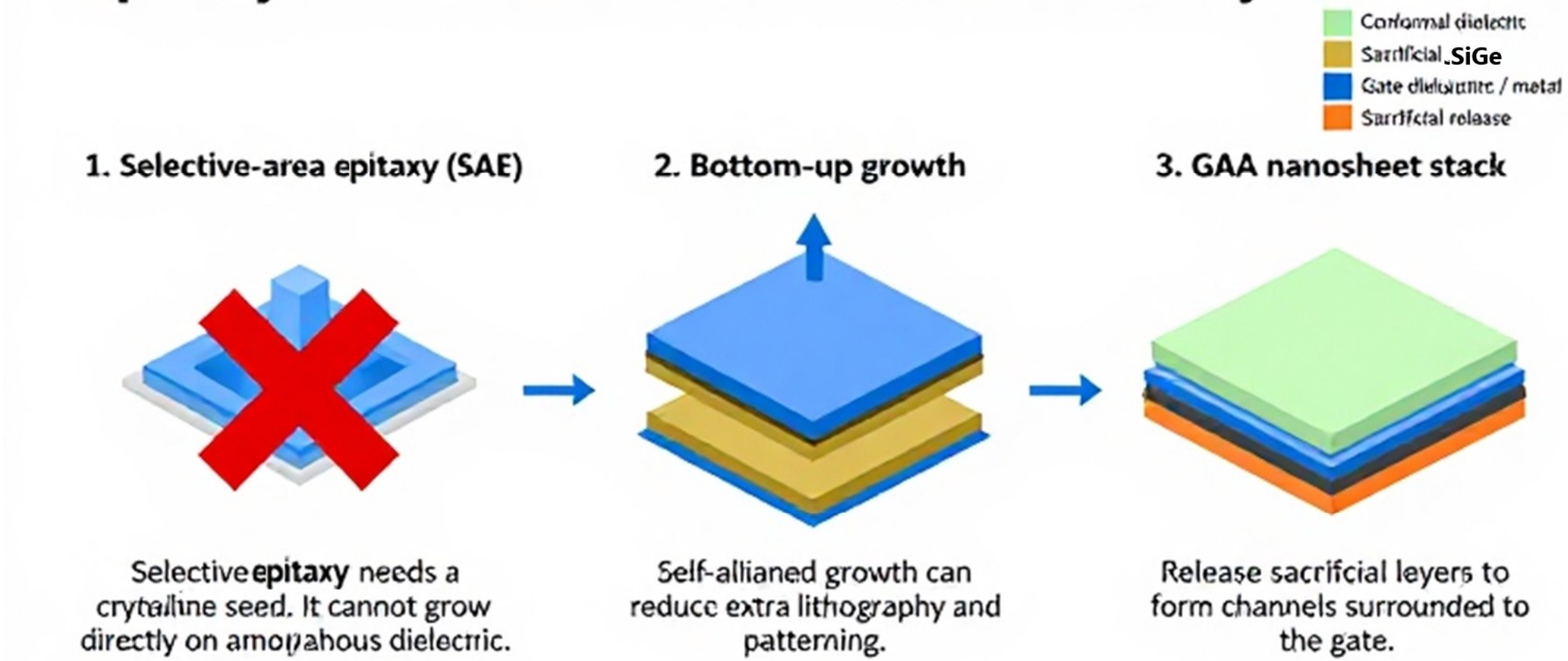
Preferred Solution



Selective Area Epitaxy

- **Selective area epitaxy (SAE)** of a SLS structure combined with sacrificial/ structural layer engineering: foundational concept in next-generation gate-all-around (GAA) nanosheet architectures
- Sub-3nm FinFET and Gate-All-Around device architectures require unprecedented critical dimension consistency and overlay precision.
- Production of 1–2 nm GAA nanosheets and nano-ribbons relies on sophisticated techniques, including Self-Aligned Quadruple Patterning and high-numerical-aperture extreme ultraviolet lithography. *Pattern Reproduction poses Significant Challenges*:
- Line-edge roughness and edge-placement deviations significantly impact manufacturing yield, frequently resulting in reduced initial yields for GAA fabrication processes.

Epitaxy-Based GAA Nanosheet Process: Key Limitation



Selective Epitaxy (Future)

Alternating stack of crystalline silicon and a dielectric material from the bottom-up without using any physical lithography masks, must be utilized **Area-Selective Deposition (ASD)** coupled with **crystalline oxide conversion**

Process phase	Material layer	Mechanism (maskless/lithography-free)
Step 1: Si epitaxy	Crystalline Si	Grown via standard chemical vapor deposition (CVD) on existing crystalline seed.
Step 2: Surface conversion	Dielectric barrier	Instead of depositing an amorphous oxide, the top atomic layers of the newly grown Si are selectively oxidized or nitrided using a self-limiting plasma process, forming a crystalline or ultra-thin, uniform dielectric interface.
Step 3: Radical desorption/reset	Nucleation inhibitor	Chemical vapors (such as chlorosilanes or specialized co-reactants) are introduced to passivate or alter the dielectric surface, preventing random particle nucleation.
Step 4: Seeded top-epi	Next Si layer	By shifting to a high-order precursor system (such as disilane or trisilane) at optimized thermal windows, the system **promotes epitaxial lateral overgrowth (ELO)** or nucleation strictly from designated peripheral crystalline borders, bypassing the un-patterned dielectric layer.

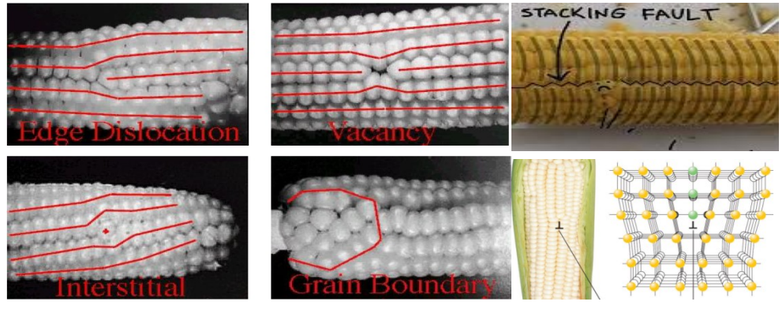
Selective Epitaxy (Future)

Engineering Trade-Offs

Crystalline oxide conversion: Need to be optimized over boundary layers, resulting in dense, uniform, and defect-free crystals.

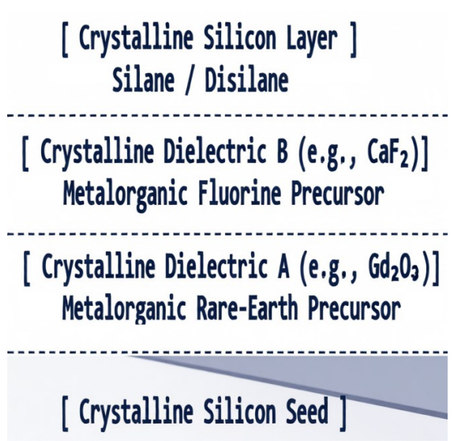
Defect Density: Growing silicon around or over dielectric boundaries without a patterned template often yields severe thermal stress and dislocation defects due to *Coefficient of Thermal Expansion* (CTE) mismatch.

Selectivity Failure: In true maskless selective epitaxy, maintaining 100% selectivity (preventing stray silicon islands from forming randomly on top of the dielectric) becomes exponentially harder need to add more layers to the superlattice stack



Selective Epitaxy (Future)

MOCVD, entire SLS can be grown sequentially in a **single run,** bypasses lithography requirement,



Gd_2O_3 align with Silicon (111) or (100) orientations. **CaF_2** lattice mismatch with Silicon 0.6% at RT.

Challenge	Impact on nanosheet superlattice	Solution / mitigation
Carbon/ organic contamination	MOCVD precursors contain organic "ligands." If they donot decompose cleanly, carbon can become trapped at the interface, degrading the dielectric's insulating properties and creating silicon defects.	Optimize the V/III ratio, use carrier gases such as H_2 or N_2, and increase the temperature as needed to fully decompose the precursors.
Thermal expansion mismatch	Silicon and oxides/fluorides expand and contract at different rates during cooling from MOCVD temp. (500–800 °C). create tensile stress and cracking across the SLS.	Use ultra-thin layers below the critical thickness and strain-compensated SLS designs.
Interfacial reactions	At high growth temp., oxygen from the dielectric can react with the growing silicon layer, forming an unwanted amorphous SiO_2 layer at interface and disrupting epitaxy.	Use low-temperature MOCVD precursors, higher-order SiH_4, enable epitaxial silicon growth at lower temp.

Selective Area Epitaxy (Power devices)

Lithography is heavily used to open windows for source/drain ohmic contacts, define sub-micron gates (often T-gates), and isolate devices. Eliminating lithography entirely requires transitioning to a **completely bottom-up, self-aligned growth regime**

Selective Area Epitaxy (SAE) to high-electron-mobility transistors (HEMTs) to eliminate standard patterning or lithography is a highly active area of research, particularly for **Gallium Nitride (GaN)** and **Indium Phosphide (InP)** high-frequency devices

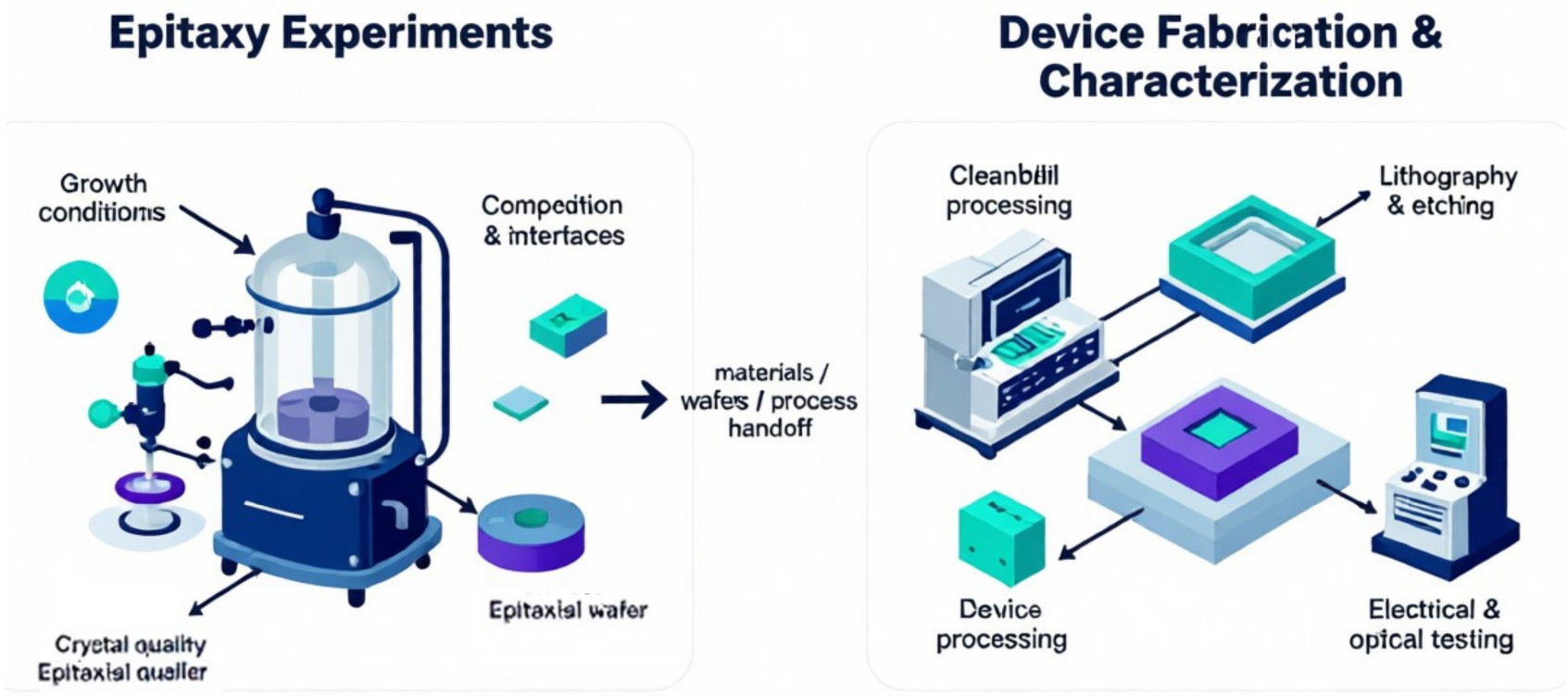
```
[ Source Contact ]       [ Re-grown Gate ]       [ Drain Contact ]
(Epitaxial n+ GaN)     (AlGaN/GaN Heterojunction)   (Epitaxial n+ GaN)
==================   ============================   ==================
-------------------------------------------------------------------
                      [ Semi-Insulating GaN Buffer ]
-------------------------------------------------------------------
                         [ Crystalline Substrate ]
```

Direct Technical Comparison

Feature	Patterning & Lithography (Traditional)	Selective Area Epitaxy (SAE)
Process nature	Subtractive: Material is deposited everywhere, then selected areas are removed by etching.	Additive: Material is selectively grown from the gas phase only on target surfaces.
Resolution limit	Limited by the wavelength of light and lens optics (for example, 13.5 nm for EUV).	Limited by atomic-scale crystal surfaces and chemical reaction rates
Material quality	Plasma etching can leave surface defects, dangling bonds, and rough edges on device channels.	Produces atomically smooth surfaces and crystal lattices with few defects.
Material freedom	Limited. Etching compound semiconductors such as GaN, SiC, or InP without damaging them is difficult.	Highly flexible for growing different materials, such as Ge on Si or AlGaN on GaN or other compound semiconductors.
Cost & throughput	EUV photomasks and multiple patterning steps are expensive, but the process handles uniform arrays well.	High initial equipment and precursor costs; throughput may be lower because precise chemical growth takes time.

*Current GAA devices production exploits combination of both techniques.

Technology Domains & Missing Info



Distinct expertise, shared materials platform

The Angstrom-Scale Scaling Crisis

- Semiconductor technology approaches from **3nm node down to the Angstrom era** (e.g., *Intel 18A/14A, TSMC A16)*
- Traditional patterning relies on top-down lithography and plasma etching, whereas **Selective Area Epitaxy (SAE)** relies on bottom-up chemical kinetics. Designing both processes at the Angstrom scale requires migrating from classical engineering models to **quantum-mechanical and atomistic simulations**.
- In nanosheet channels and HEMT heterojunctions under 5 nm thick, electrons behave *purely as waves* rather than classical particles.
- Continuum physics models (Synopsys & Silvaco TCAD) completely break down at dimensions of only several atomic layers, a single atom's displacement can cause transistor failure.
- Atomistic modeling tools will be crucial to accurately predict **source-to-drain direct quantum tunneling** and gate leakage

Kinetic Selectivity and Nucleation Time

In maskless selective epitaxy, maintaining perfect selectivity is a race against time. Precursor molecules must deposit on the seed area but desorb from the dielectric area before they form a random atomic nucleus.

- **The Need:** Engineers must know the precise **resident time** (how long they can run the MOCVD gas before a defect forms).
- To develop Angstrom-scale processes via pure physical trial-and-error in a cleanroom is financially unsustainable.
- A single advanced test mask set **costs millions of dollars**, and a full wafer **processing cycle takes months**.
- Atomistic modeling reduces this loop to days, serving as a virtual sandbox to test new chemical precursors, thermal parameters, and crystal configurations prior to physical execution.

Requirements

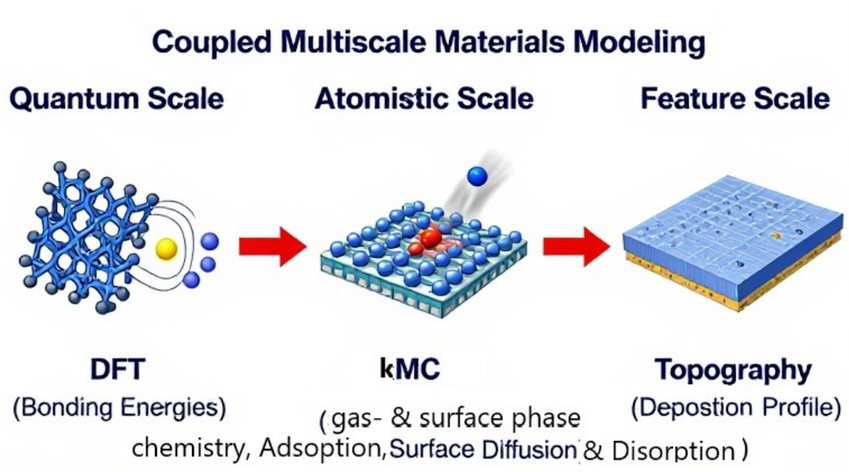
- **Simulation Tool: Kinetic Monte Carlo (kMC)** and **Density Functional Theory (DFT)**. These models simulate individual precursor molecule collisions, surface migrations, and chemical bond formations at specific crystal coordinates.

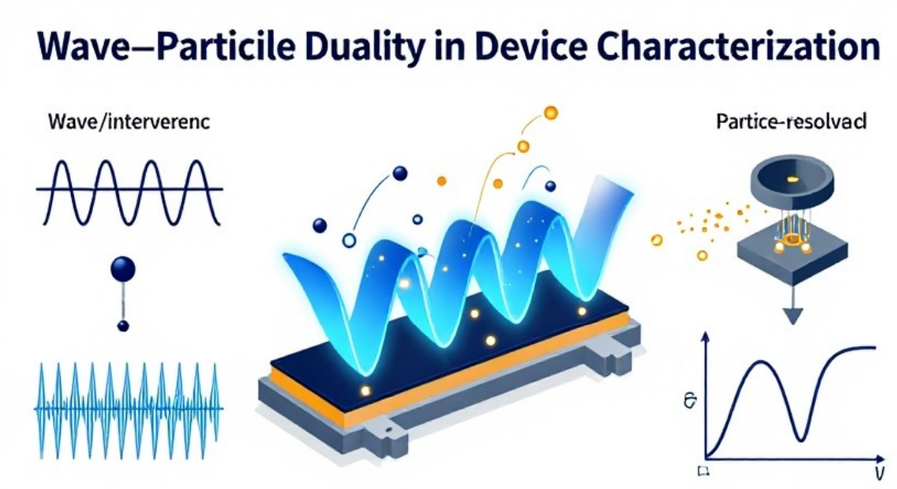
Requirement of Hierarchical Simulation Stack Toolkit for Advanced Technology

[Quantum Scale] -->	[Atomistic Scale] -->	[Feature Scale]
DFT	kMC & MD	Topography
(Bonding Energies)	(Surface Diffusion)	(Deposition Profile)
Quantum mechanical bonding energies of MOCVD precursors on specific crystal facets	**Real-time pathing of surface diffusion, incubation times, crystal defect generation, and atomic strain.**	**3D shape evolution of the nanosheet or HEMT profile inside the reactor chamber over time.**

TNL Organization and Mission

Our organization constitutes a unified body committed to providing atomistic-scale precision modeling and simulation capabilities designed to achieve measurable outcomes for next-generation semiconductor device technologies, delivered through our proprietary TNL TCAD software platform.





Organization's Profile (Semiconductor)

Leading TCAD: innovation and pioneering design starts from the wafer growth to material & device characterization

- *Atomistic Scale* Technology Computer-aided design (TCAD) tools
  - ❑ ***Epitaxy Growth Solution***
  - ❑ **Material Characterization**
  - ❑ **Device Characterization**

Strengths:

- ➢ Self Funded since its inception
- ➢ PhD & Masters Team Members
- ➢ Collaborators from Fabs
- ➢ Successfully delivered Technologies

KEY Milestones Achieved

- TNL incorporated — July, 2015
- Q4 2017 — Successfully delivered Design Guideline on InGaAs IR detector Technology to **SSPL, DRDO**
- Successfully delivered Dosimetry Tech to **SAC , used in next Indian Lunar Mission** — Q4 2021
- Delivered **III-V Nitrides MOCVD Epitaxy** solution to **SCL Mohali, Ministry of Electrnics & information Technology (MEITY)** — Q4 2024
- Signed Partnership to optimize **III-V Nitrides MOCVD Epitaxy solution** ; **Defense Research & Development Organization (DRDO), India** — Q1 2025
- Q2 2025 — Signed NDA to optimize **III-V Nitrides & 2D material Epitaxy processes and Reactors; AIXTRON**
- Signed NDA to optimize **Si & SiGe Epitaxy processes: QUANTUMSEMI, USA** — Q2 2025
- Q2 2025 — Signed NDA to optimize **PECVD Epitaxy processes ; INFINEON**
- Signed Contract to enhance **Diamond MPCVD Epitaxy growth rates** ; **NEO AEON DIAMOND** — Q2 2025

Our Partners

Leading TCAD: innovation and pioneering design starts from the wafer growth to material & device characterization

Many More ……..

Atomistic TNL TCAD Full Flow



Wafer Growth

- MBE
- MOCVD
  - INJECTOR
  - Showerhead
- CVD

Material Characterization

- Full Electronic Band Structure
  - Carrier Field Mobility
  - THz Spectroscopy

Device Characterization

- Particle /wave duality
  - BTE/Wigner
  - Monte Carlo

Outputs

Lattice Parameter | Defects | Band Structure | DOS | Transfer Characteristics | Atomistic | Etc

Strain | Roughness | Carrier Mobility | Conductivity | Bulk/Nano | Quantum Confinement

TNL

DISCUSSION



MOCVD/MOVPE User: Have you thought any time about:

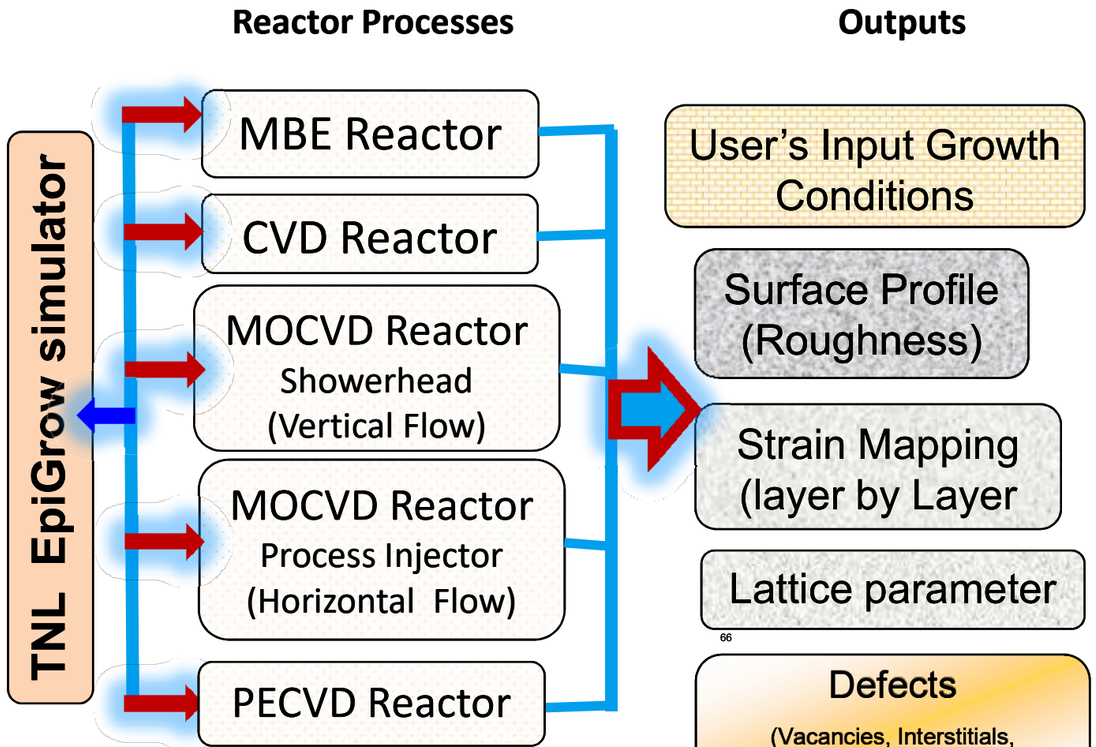
- ❑ Contribution of variation in distance between substrate and gas inlet
- ❑ What about Substrate Temperature Uniformity
- ❑ Temperature Gradient inside chamber
- ❑ Role of Chamber Pressure
- ❑ Reactor Chamber Geometry and Volume Role
- ❑ Chemical Kinetics
  - ❑ Gas Phase & Surface phase Chemistry
- ❑ Up and Down Diffusion of various undesired foreign atoms
- ❑ Low Temperature Growth
- ❑ High Temperature Growth
- ❑ Various Energy Barriers (How 2D, 3D growth occur) and so many other aspects ….

TNL Epitaxy Solutions



TNL-EpiGrow simulator

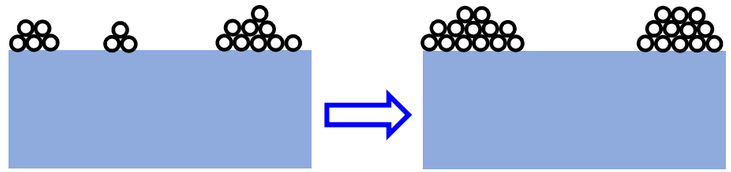
- ❑ Industry Standard
- ❑ Calibrated against Experiments
- ❑ Reactor's geometry dependent
- ❑ Gas- & Surface-Phase Chemistry
- ❑ NIST Database (Enthalpy, Entropy)
- ❑ User's define reactions and paths
- ❑ Map each atom/molecule inside reactor
- ❑ Extract growth mode, lattice parameters, strain, defects etc.
- ❑ DOE for Optimization
- ❑ Accuracy upto a monolayer
- ❑ ***Cost-economical Epitaxy solution***
- ❑ Flexibility to include Patterned substrate



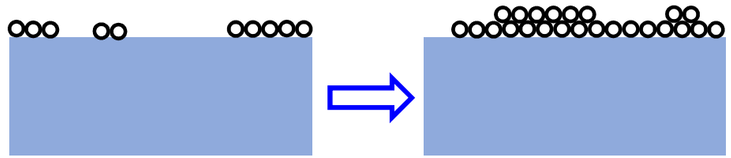
Growth mode

Energy dependent

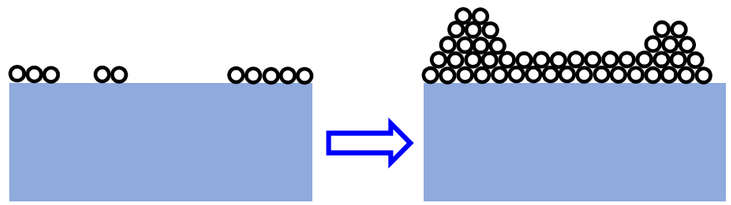
- Island growth from small clusters that nucleate on the surface and grow in three dimensions, this growth mode occurs when the atoms in deposit are more strongly bound to each other than to the substrate and common in heteroepitaxial growth.
- The atoms are more strongly bound to the substrate than to each other, the growth from the initial nucleus will occur only in two dimensions and this will result in a layer growth, common in homoepitaxial growth.
- A combination of the layered and island growth is the Stranski-Krastanov growth mode



Island (*Volmer-Weber*)



Layer (***Frank-Van der Merwe***)



Stranski-Krastanov

EXTRACTABLE



1. Lattice Paramters :

- ❑ 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

Proven Processes

MOCVD Process / Reactors	CVD Reactor	(AIX 200/4, and G5+) Horizontal Flow Reactor	(CCS-Showerhead) Vertical Flow Reactor	Proven Reliability
Si, SiGe, SiC Epitaxy	YES			Fab
MoS_2 and WS_2	YES			Fab
III-V nitrides binary & ternary Epitaxy on Sapphire, SiC and Si	**Yes**			**Fab**
Pre-Nitridation: NH_3 pre-flow, buffer layers strain profile with SiN_x patches	Yes	Yes		Fab
Pre-Aluminization: TMAl Pre-flow	Yes			Fab
TMAl pre-flow impact on buffer layers strain profile & Al Diffusion	Yes			Fab
Role of Range of Pressure & Temp	Yes			Fab
Mg, Fe Dopings and C contamination	Yes	Yes		Fab
III – As, Sb, P based epitaxy		YES		FAB

CVD Reactor Deposition Process

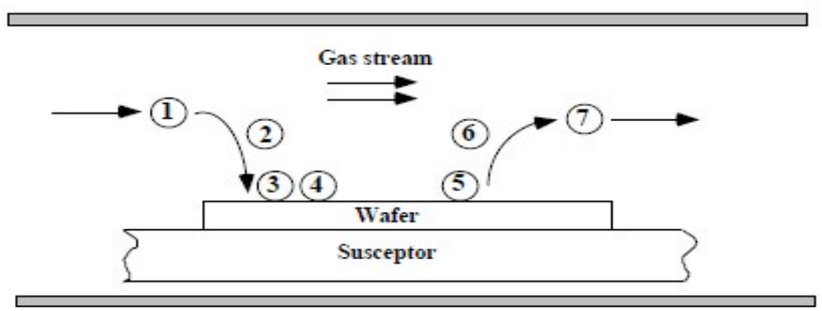
CHEMICAL KINETICS



React		$Log_{10}A$	α	E
G-1	$SiH_4 \leftrightarrow SiH_2 + H_2$	9.49	1.70	54710
G-2	$Si_2H_6 \leftrightarrow SiH_4 + SiH_2$	10.26	1.70	50200
G-3_f	$HSiSiH_3 + SiH_4 \leftrightarrow Si_2H_6 + SiH_2$	14.24	0.40	8900
G-4	$Si_2H_6 \leftrightarrow H_2 + HSiSiH_3$	9.96	1.80	54200
G-5	$HSiSiH_3 \leftrightarrow H_2SiSiH_2$	13.40	−0.20	5380
G-6_f	$HSiSiH_3 + H_2 \leftrightarrow SiH_2 + SiH_4$	13.97	0.00	4092
A-1	$SiH_4 + 2\sigma \rightarrow SiH_3^* + H^*$	19.06	0.5	3000
A-2	$SiH_3 + \sigma \rightarrow SiH_2^* + H^*$	17.64	—	27000
A-3	$2SiH_2^* \rightarrow 2SiH^* + H_2$	24.38	—	45000
A-4	$SiH_2 + \sigma \rightarrow SiH_2^*$	11.76	0.5	0
A-5	$SiH^* \rightarrow Si(s) + \frac{1}{2}H_2 + \sigma$	11.90	—	47000
A-6	$2H^* \rightarrow H_2 + 2\sigma$	22.11	—	43000
A-7	$H_2 + 2\sigma \rightarrow 2H^*$	11.36	0.5	17250

METHODOLOGY: CVD PROCESS





1. Transport of reactants to the deposition region.
*2. Transport of reactants from the main gas stream through the boundary layer to the wafer surface.
*3. Adsorption of reactants on the wafer surface.
*4. Surface reactions, including: chemical decomposition or reaction, surface migration to attachment sites (kinks and ledges); site incorporation; and other surface reactions (emission and redeposition for example).
*5. Desorption of byproducts.
6. Transport of byproducts through boundary layer.
7. Transport of byproducts away from the deposition region.

METHODOLOGY: CVD PROCESS



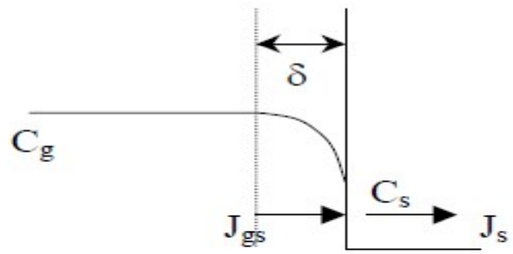
$J_{gs} = h_g (C_g - C_s)$

h_g gas phase mass transfer coefficient

$J_s = k_S C_s$

k_S surface reaction rate constant

$J_s = J_{gs}$ gives $C_s = C_g / (1 + k_s / h_g)$



Film growth rate $g = J_s/N_0 = [k_s h_g/(k_s + h_g)](C_g/N_0)$

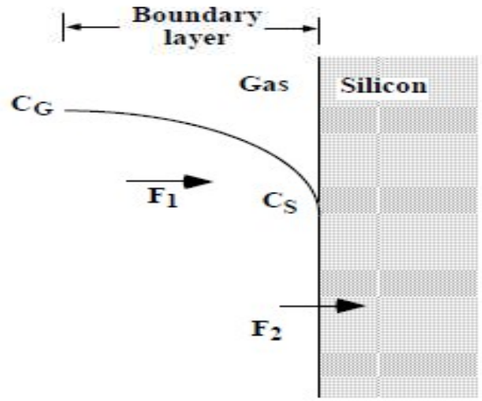
(N_0=atomic density/unit vol. of film)

Mass Transfer (diffusion) rate control $h_g << k_s$

Reaction (kinetic) rate control $k_s << h_g$

METHODOLOGY: CVD PROCESS





F_1 = diffusion flux of reactant species to the wafer
= mass transfer flux, step 2

$$F_1 = h_G(C_G - C_S) \quad (4)$$

where h_G is the mass transfer coefficient (in cm/sec).

F_2 = flux of reactant consumed by the surface reaction
= surface reaction flux, steps 3-5

$$F_2 = k_S C_S \quad (5)$$

where k_S is the surface reaction rate (in cm/sec).

In steady state: $F = F_1 = F_2$ (6)

Equating Equations (4) and (5) leads to $$C_S = C_G\left(1 + \frac{k_S}{h_G}\right)^{-1} \quad (7)$$

The growth rate of the film is now given by $$v = \frac{F}{N} = \frac{k_S h_G}{k_S + h_G}\frac{C_G}{N} = \frac{k_S h_G}{k_S + h_G}\frac{C_T}{N}Y \quad (8)$$

where N is the number of atoms per unit volume in the film (5×10^{22} cm^{-3} for the case of epitaxial Si deposition) and Y is the mole fraction (partial pressure/total pressure) of the incorporating species.

METHODOLOGY: CVD PROCESS



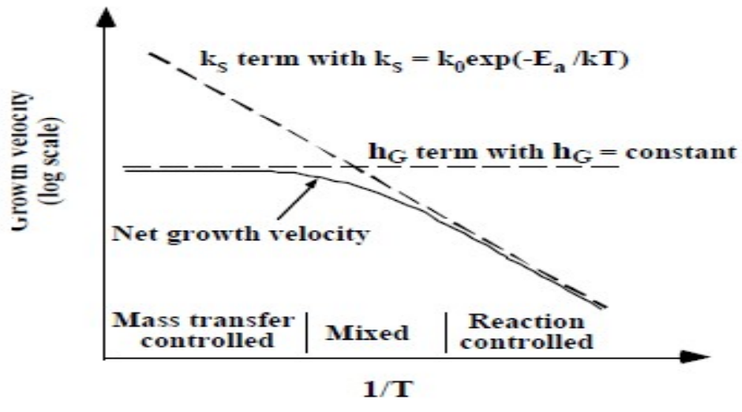
$$v = \frac{F}{N} = \frac{k_S h_G}{k_S + h_G}\frac{C_G}{N} = \frac{k_S h_G}{k_S + h_G}\frac{C_T}{N}Y$$

1. If $k_S << h_G$, then we have the surface reaction controlled case:

$$v \cong \frac{C_T}{N}k_S Y \qquad (9)$$

2. If $h_G << k_S$, then we have the mass transfer, or gas phase diffusion, controlled case:

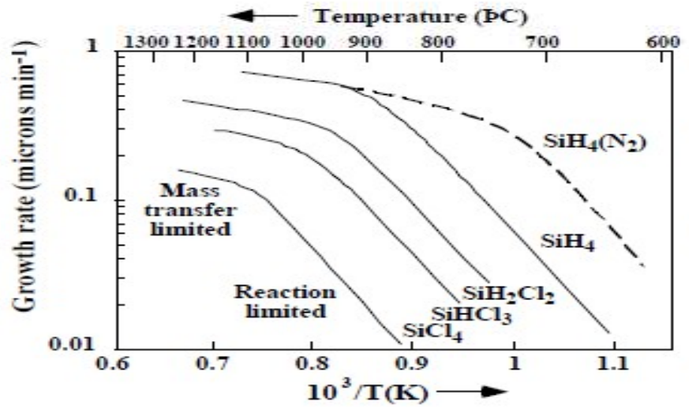
$$v \cong \frac{C_T}{N}h_G Y \qquad (10)$$



- The surface term is Arrhenius with E_A depending on the particular reaction (1.6 eV for single crystal silicon deposition).
- h_G is ≈ constant (diffusion through boundary layer).
- As an example, Si epitaxial deposition is shown in the next slide (at 1 atm. total pressure). Note same E_A values and h_G ≈ constant. Rate is roughly proportional to $(\text{mol. wt.})^{-1/2}$.

METHODOLOGY: CVD PROCESS

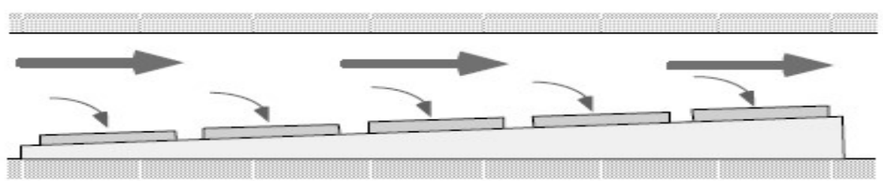




Key points:

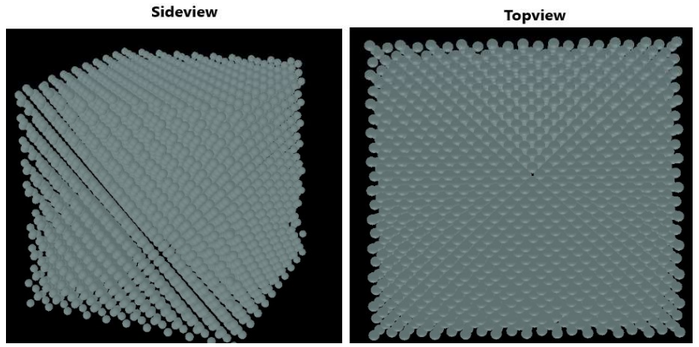
- k_S limited deposition is VERY temp sensitive.
- h_G limited deposition is VERY geometry (boundary layer) sensitive.
- Si epi deposition often done at high T to get high quality single crystal growth. ∴ h_G controlled. ∴ horizontal reactor configuration.
- h_G corresponds to diffusion through a boundary layer of thickness δ_S .

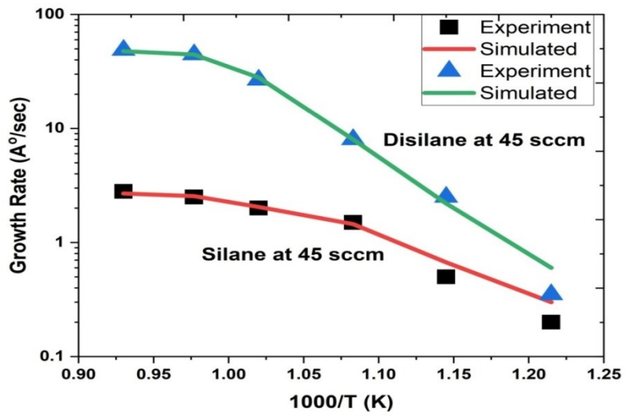
Assumed $F_1=h_g(C_g-C_s)$
Fick's Law for the boundary layer → $F_1 = -D_g \frac{\partial C}{\partial x} = \frac{D_g}{\delta_s}(C_g - C_s)$



- But typically δ_S is not constant as the gas flows along a surface. ∴ special geometry is required for uniform deposition.

CASE STUDY : Si CVD PROCESS

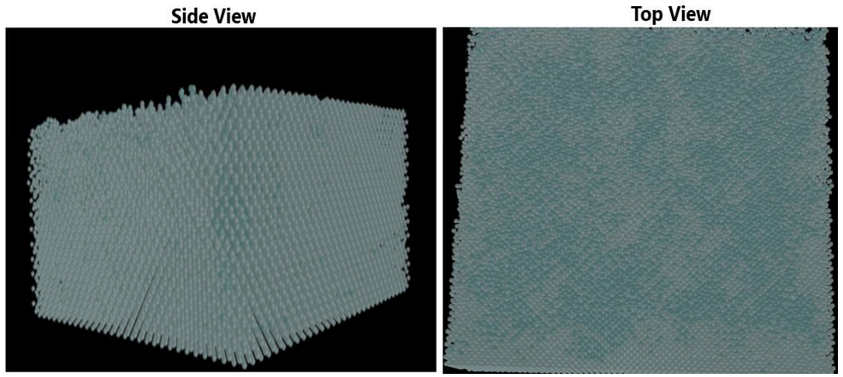


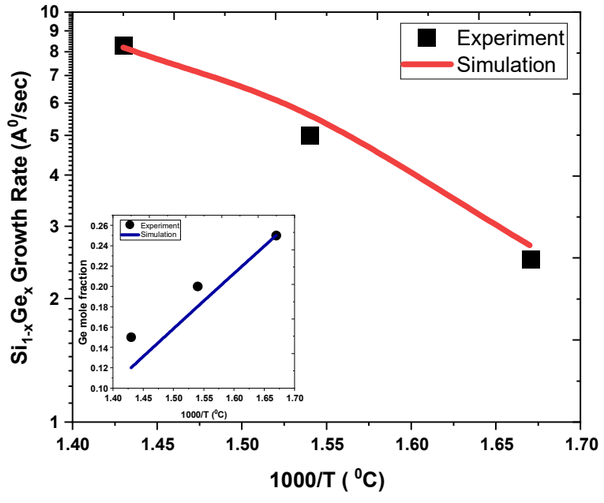


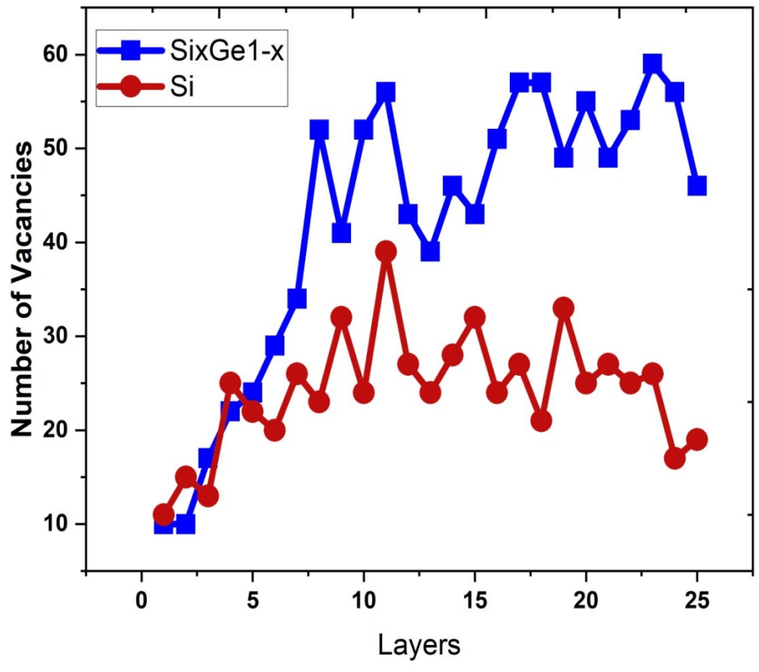
Parameters	Si	Si_xGe_{1-x}
Chamber Temperature (°C)	550 - 800	600 - 700
Chamber Pressure (Torr)	10	80
Cross Sectional Area (cm^2)	12	12
Length of Chamber (cm)	100	100
Distance between Substrate and Edge (cm)	1.0	1.0
Precursors	SiH_4/Si_2H_6	SiH_4 & GeH_4
Precursors Flow Rate (sccm)	45	10 & 1
Carrier Gas	H_2	H_2
Carrier Gas Flow Rate (sccm)	10000	10000
Substrate Temperature (C)	800	800
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 Energy (eV)	0.05	0.05
No. of Interactive Elements	1	1

- *Mater. Adv., 2024, 5, 2110–2119*

CASE STUDY-I : **SiGe** CVD PROCESS



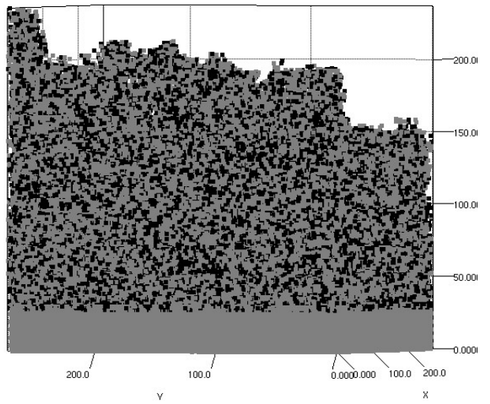


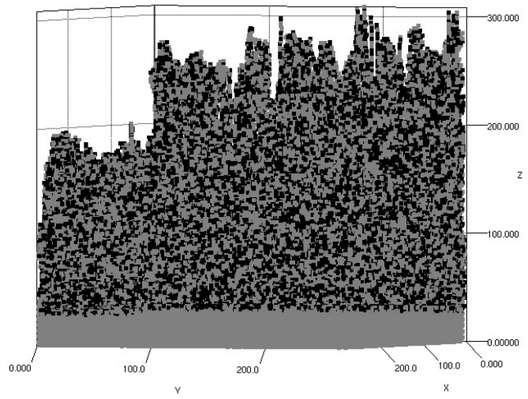


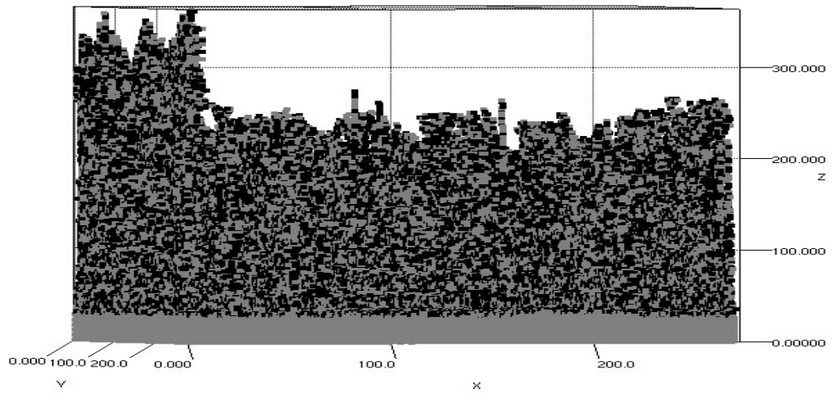
- *Mater. Adv., 2024, 5, 2110–2119*

SiGe CVD Process

Orientation	Temp	Chamber Press.	Sr. Energy	Sch. Barrier	IncorBarrier	Des. Barrier	GeH_4/SiH_2Cl_2 Ratio
Si 100	550	20 mbar	2 eV	0.1 eV	0.1 eV	3 eV	0.1
							0.15
							0.2
Si 100	600						0.05
							0.1
Si 100	650						0,1

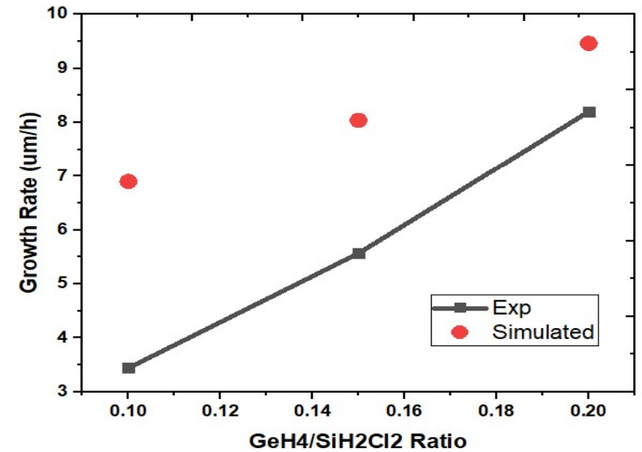




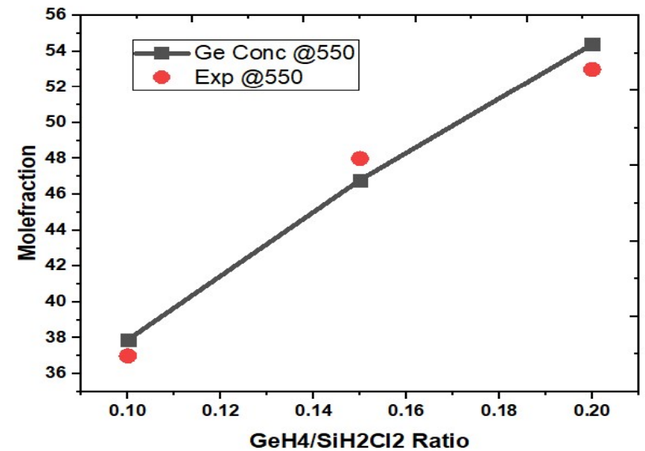


CASE STUDY-II : **SiGe** CVD PROCESS

Ratio	Lattice Parameters (°A)			Growth Rate (°A/s)	Dislocations Density (A^{-2})	Vacancies (A^{-3})
	a	b	c			
0.1	5.29	5.39	7.14	1.15	$1.91x10^{-4}$	991
0.15	5.47	5.42	5.78	1.34	$1.75x10^{-4}$	1096
0.2	5.34	5.40	6.19	1.57	$1.54x10^{-4}$	1323

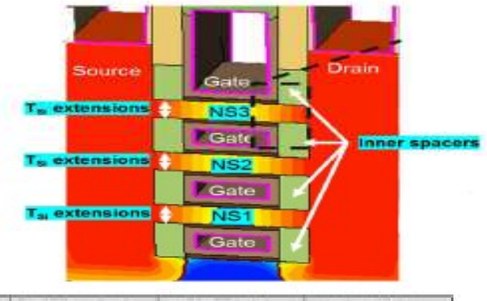


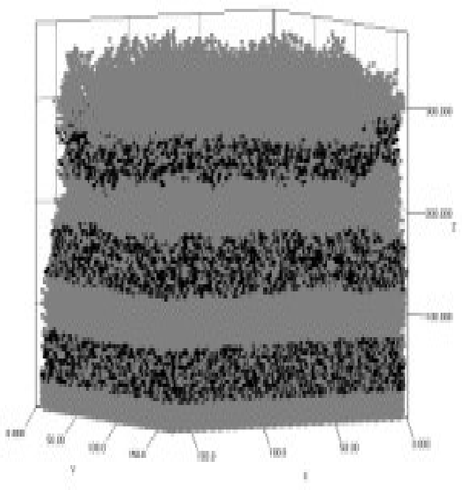
Ratio	Lattice Parameters (°A)			Growth Rate (°A/s)	Dislocations Density (A^{-2})	Vacancies (A^{-3})
	a	b	c			
0.05	5.34	5.37	5.86	2.25	$1.48x10^{-4}$	1426
0.1	5.44	5.43	5.85	2.57	$1.27x10^{-4}$	1357
0.1@650	5.47	5.34	5.90	4.83	$9.95x10^{-5}$	1432

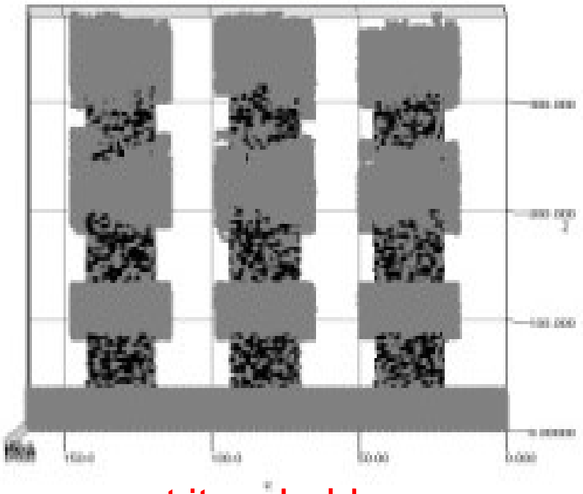


III: Si/SiGe Depo & Etch

- Advance node devices epitaxy without any limitation
- Chemistry based Angstrom-scale precision Dry Etching with spacer filling







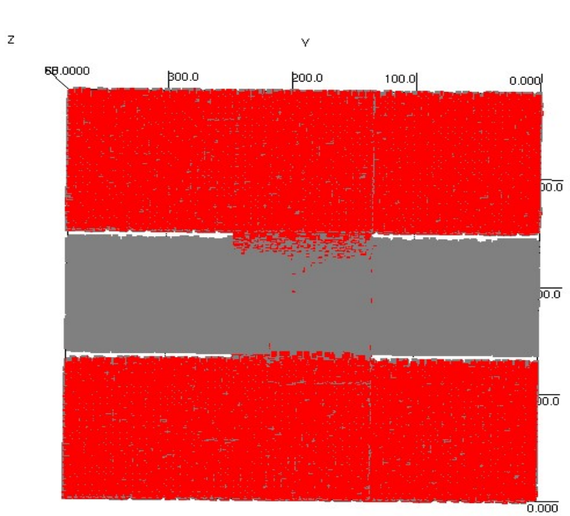
❖ We have started this project with ***TEL***, but due to funding issue we put it on hold.

❖ TNL is looking for interested Industry partner to start this project again.

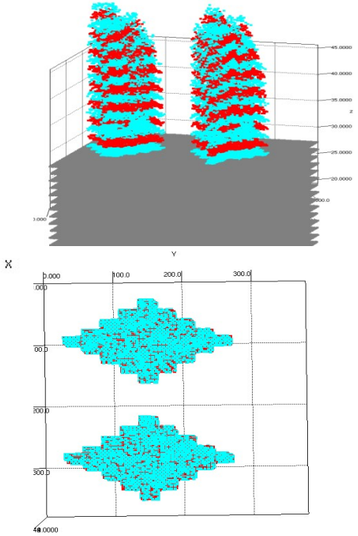
SELECTIVE EPITAXY



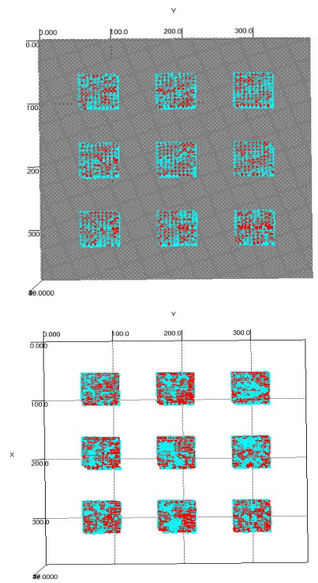
Simulation Process utilizes a mask (containing the exposed "seed" windows info of the substrate in .txt format) , and deposit the require patterned on a substrate.
The selective epitaxy simulation supports MBE, CVD and MOCVD reactors processes



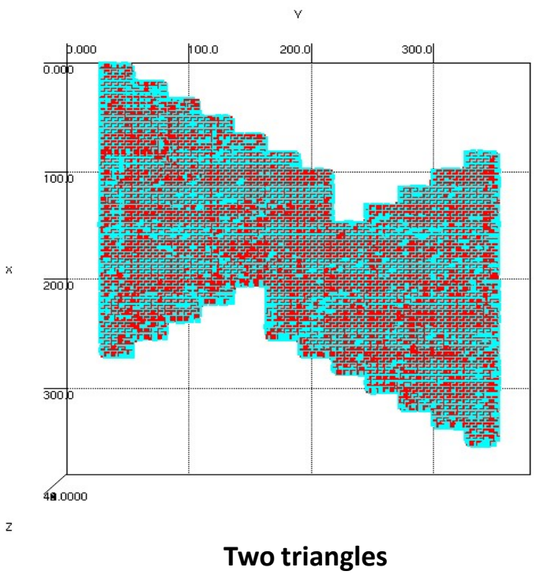
FinFET



Nano Patterns (Nanowire)

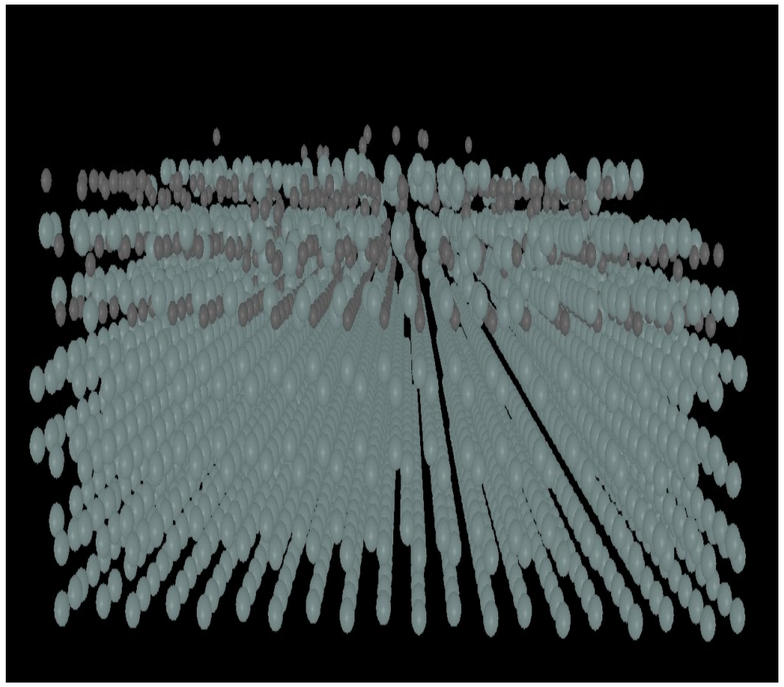


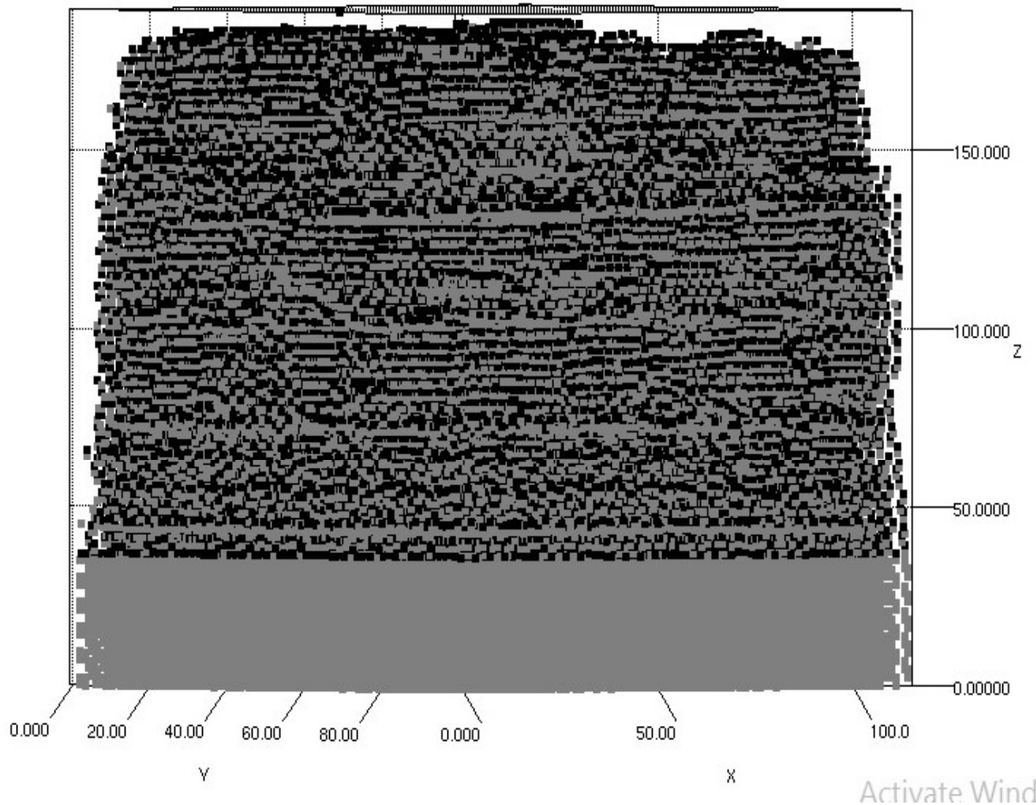
Nano Patterns (Quantum Dots)



Two triangles

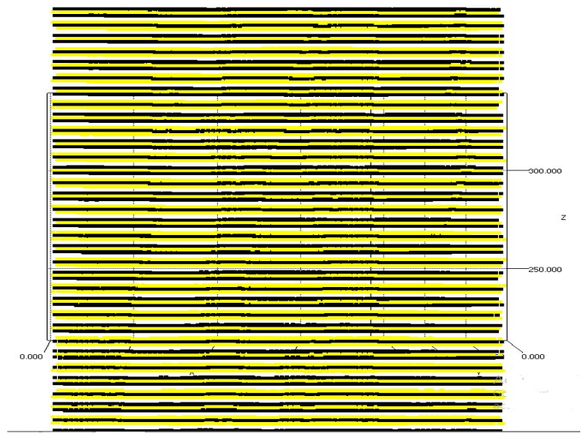
SiC CVD Process

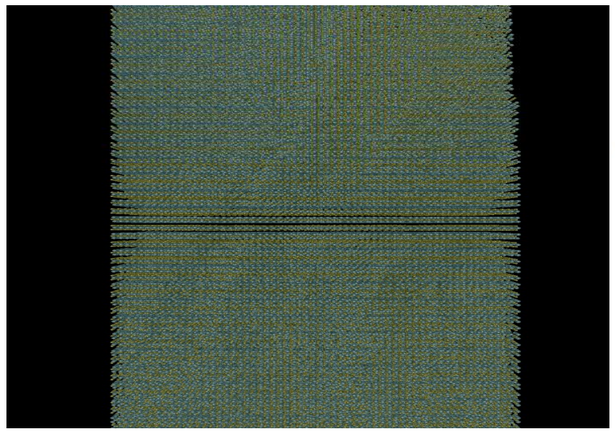


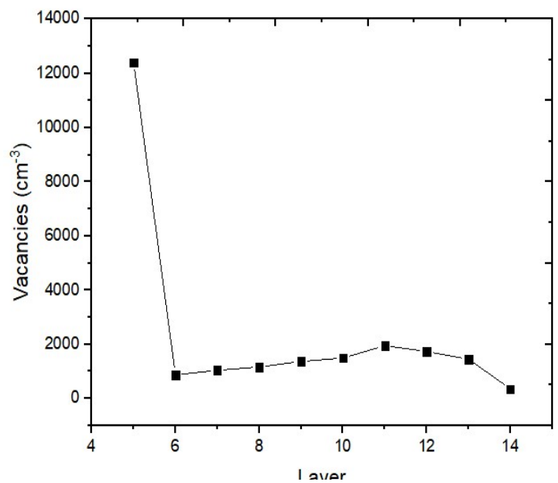


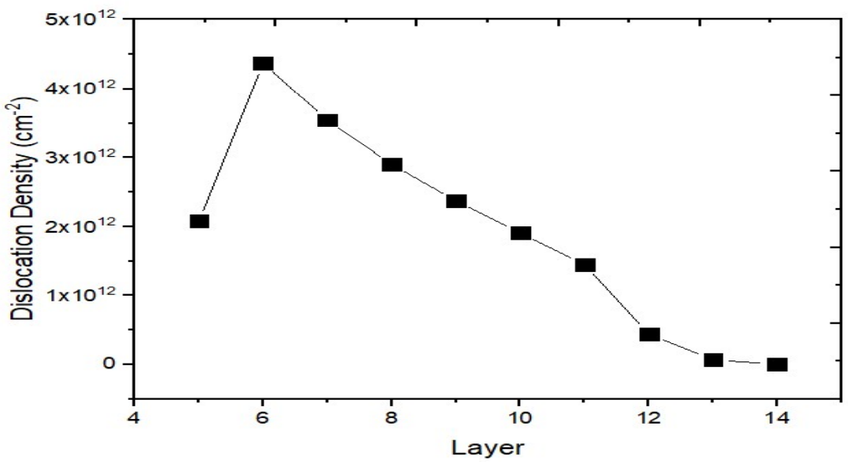
Activate Wind

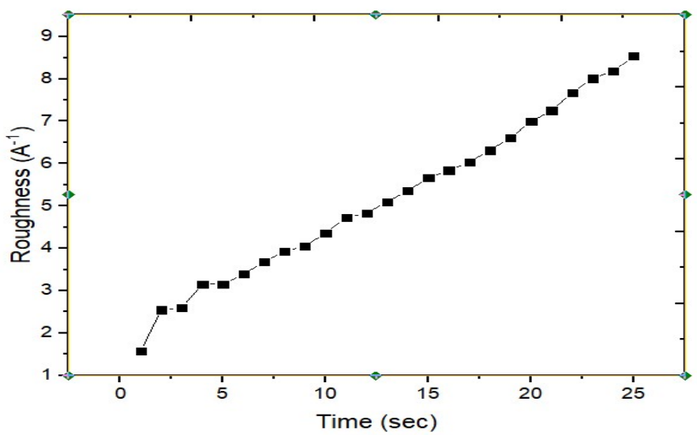
MoS_2 Epitaxy





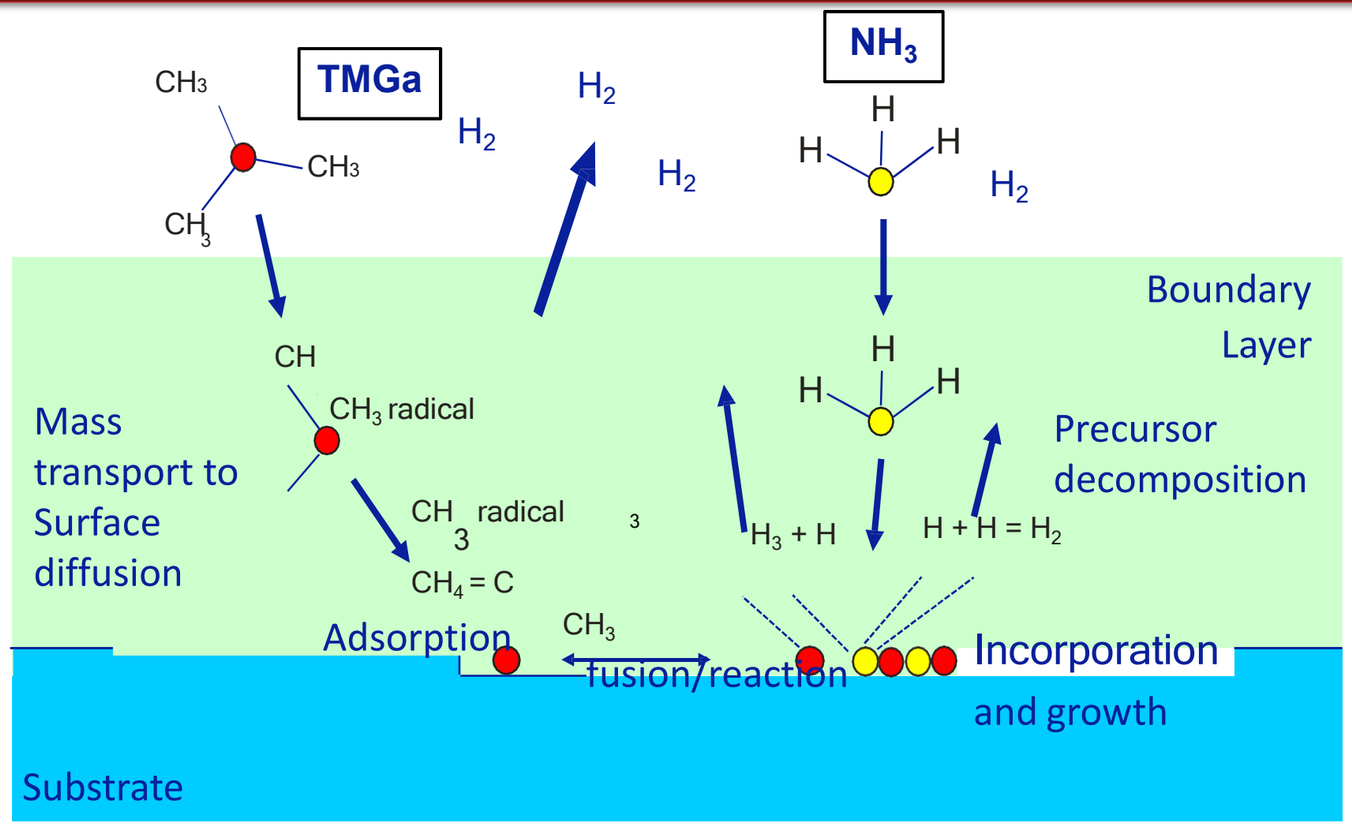






TNL Epitaxy Solution

III-N AIX-Series,G5, G10, CCS MOCVD Reactors

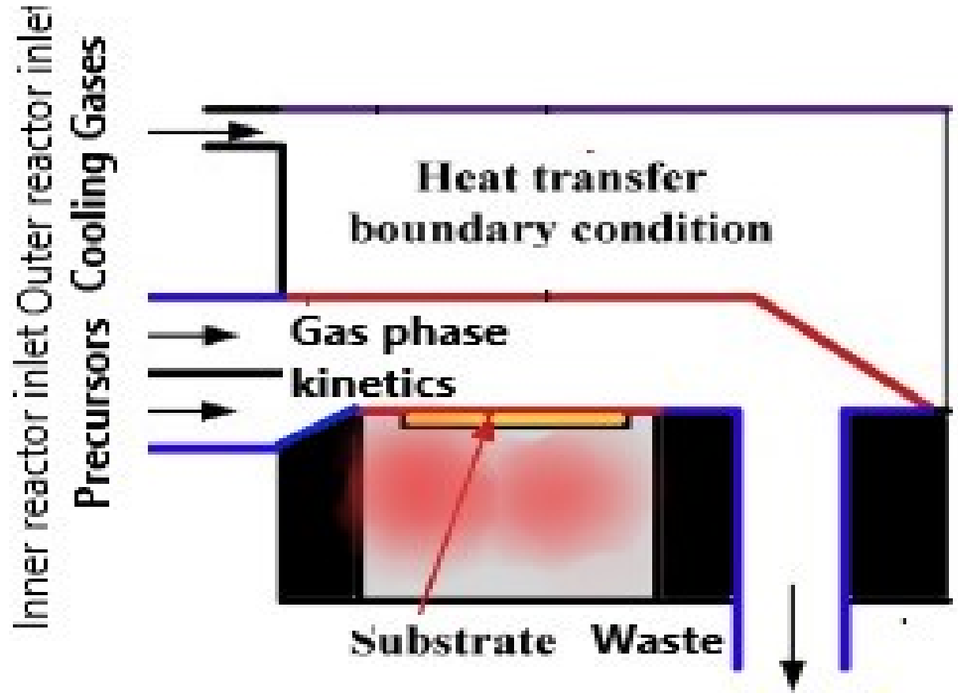


PLANETARY MOCVD PROCESS



Planetary MOCVD architecture implemented in ***TNL-EpiGrow*** **simulator** equivalent to the **horizontal flow MOCVD reactor**.

Inlet of the reactor is divided into parts by a separator through which the group III, V precursors and carrier gases can be fed into the inlets 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 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.

SHOWERHEAD MOCVD PROCESS



The impact of the geometry of the showerhead MOCVD reactor is considered by utilizing a showerhead flange equipped with numerous small holes of radius r, which directs the reactant gases vertically onto the substrate. The vertical distance between the showerhead and the substrate is defined as the ceiling height, H_C, while the radius of the reaction chamber, R, is employed to calculate the residence time, t_{res}

$$t_{res} = -\frac{H_c}{v_{in}} ln \frac{\delta}{H_c} + \frac{\delta^2}{4D}$$

The estimation of the boundary layer thickness in stagnation flow is referenced in[28].

$$\frac{\delta}{H_c} = 3\sqrt{\frac{\pi R^2 \gamma_{STP}}{V_m F_{in} H_c}}$$

γ_{STP} represents kinematic viscosity, F_{in} denotes the molar flow, and V_m indicates the molar volume at standard temperature and pressure (STP).

SHOWERHEAD MOCVD PROCESS



- Reactor geometry: ratio of the diffusion length and the chamber radius (L_d/R decides radial mass transport, while the ratio of the diffusion length and the ceiling height (L_d/H_C dominates axial (vertical) mass transport of the reactor.
- The relevant dimensionless number i.e. **L_d/R** or **L_d/H_C** are;
  - if much larger than 1, then diffusion dominates transport;
  - if the dimensionless number is much smaller than 1, then convection dominates
  - if the number is comparable to 1, both diffusion and convection are important.
- Design of Experiments (DOE) help to optimize the distance between showerhead flange and substrate
- Axial and radial velocity components of gases

SHOWERHEAD MOCVD PROCESS



(a) For $\frac{\delta}{H_c} \geq 1$, convection has a minimal impact on the vertical transport of mass and momentum.

(b) For $\frac{\delta}{H_c} \leq 1$, the boundary layers are relatively thin in comparison to the height of the chamber, resulting in stagnation flow.

(c) If both the flow rate and ceiling height are increased, convection will become increasingly significant in the vertical transport process.

- ❑ Residence time < consumption time, the mechanism is known as surface limited, resulting in good film uniformity but low utilization efficiency.
- ❑ Consumption time < residence time referred as "mass transport limited", leading to poor deposition uniformity due to concentration gradients.
- ❑ High temperatures, surface reaction rates are faster than transport rates, making "mass transport limited" deposition typical.
- ❑ The residence time is crucial in assessing mass transport, as longer gas residence times indicate lower transport rates and film growth rates, but can also lead to harmful parasitic reactions.

CHEMICAL KINETICS



Two separate approaches are inbuilt to handle the gas- and surface-phase chemical kinetics:

- **Fugacity based approach**
  (To measure of deviations of a real gas from ideal gas behavior)
- Modified Arrhenius approach (*Equivalent to CHEMKIN, Cantera*)
  (Prefactor A, Activation Energy E_a, temperature Exponent n)

Depending upon USER'S choice, both techniques generates similar results.

TNL Chemical Kinetics



- *Thermodynamics of chemical reactions uses the equilibrium condition depending upon the forward and reverse reactions rates.*
- *Thermodynamics provides much vital information to the kineticist and to the reactor designer.*
- *The basic step in determining the economic feasibility of producing a given material from a given reactant feed stock should be the determination of the product yield at equilibrium at the conditions of the reactor outlet.*
- *Each of the individual reactions involves the formation of a compound from its elements or the decomposition of a compound into those elements.*
- *The standard enthalpy change of a reaction that involves the formation of a compound from its elements is the determination of the standard Gibbs free energy and enthalpy of formation of its compounds.*
- *If ΔH^0 -negative, exothermic; if ΔH^0 - positive, reaction is endothermic.*
- *Effect of temperature on ΔH^0*

TNL Chemical Kinetics - I



TNL-Chemical Kinetics package is designed to work with NIST database i.e. seven coefficients are needed for each of two temperature ranges. These fits take the following form:

Constant pressure heat capacity

$$\frac{C_{Pk}^0}{R} = a_{1k} + a_{2k}T + a_{3k}T^2 + a_{4k}T^3 + a_{5k}T^4$$

Temperature Dependent Enthalpy

$$\frac{H_k^0}{RT} = a_{1k} + \frac{a_{2k}}{2}T + \frac{a_{3k}}{3}T^2 + \frac{a_{4k}}{4}T^3 + \frac{a_{5k}}{5}T^4 + \frac{a_{6k}}{T}$$

Temperature Dependent Entropy

$$\frac{S_k^0}{R} = a_{1k}\ln T + a_{2k}T + \frac{a_{3k}}{2}T^2 + \frac{a_{4k}}{3}T^3 + \frac{a_{5k}}{4}T^4 + a_{7k}$$

Gibb's Free Energy

$$G_P^0 = H_k^0 - TS_k^0$$

TNL Chemical Kinetics



Fugacity Approach : An innovative Technique

For a system at equilibrium,

$$\Delta G^0_{k,i} = -RT \ln\left(\prod_i a_i^{\nu_i}\right)$$

$a_i^{\nu_i}$

Here, - activities of the various species.

Equilibrium constant

$$k_i = e^{-\Delta G_i^0/RT}$$

Including Role of Pressure

$$f_i = y_i \left(\frac{f}{P}\right)_i P$$

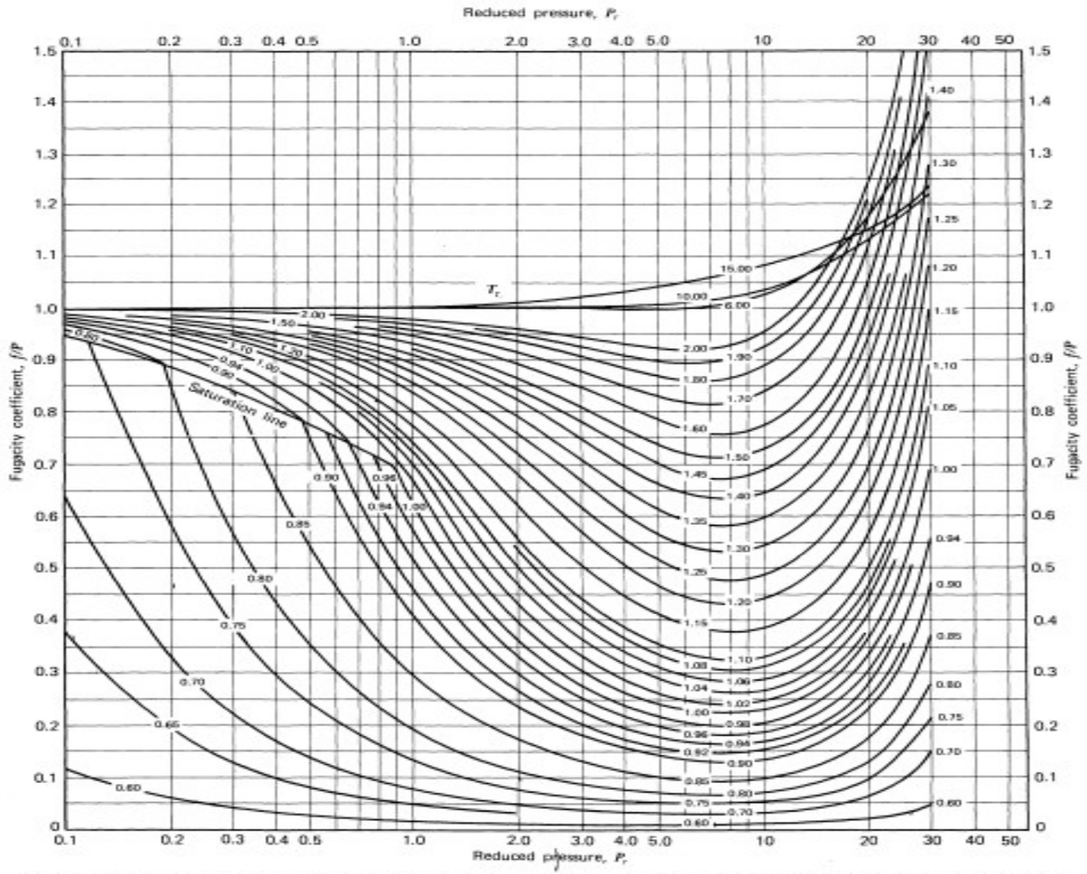
y_i is the mole fraction i in the gaseous phase, f is the fugacity of pure component 'I' evaluated at the temperature and total pressure (P) of the reaction mixture. $(f/P)_i$ is the fugacity coefficient.

TNL Chemical Kinetics

$$k_i = K_p K_{f/p}$$

For cases where the gases behave ideally, the fugacity coefficients may be taken as unity and the term K_P equated to k_i.

The fugacity coefficients {f/P) for the various species may be determined from the generalized chart if one knows the *critical temperature and pressure* corresponding to the species in question.



(Reprinted from *Chemical Process Principles Charts*, Third Edition, by O. A. Hougen, K. M. Watson, and R. A. Ragatz. Copyright 1964. Reprinted by permission of John Wiley and Sons, Inc.)

TNL Chemical Kinetics - II



In this method, forward rate constants for the i[th] reaction are determined using a modified Arrhenius equation

$$k_{fi} = AT^{n}\exp\left(-\frac{E_a}{R_c T}\right)$$

The prefactor A, which has units that vary based on the reaction order, encompasses details about the random motion of molecules as they undergo vibration, rotation, and translation within the reactor environment, contributing to the calculation of the molecules' thermal energy.

The reverse rate constants

$$k_{ri} = \frac{k_{fi}}{K_{ci}} \qquad \text{where,} \qquad K_{ci} = K_{pi}\left(\frac{P_{atm}}{RT}\right)^{\Sigma_{k=1}^{K}\nu_{ki}}$$

K_{ci} is the equilibrium constant in concentration units and easily determined from the thermodynamic properties in pressure units; P_{atm} denotes a pressure of 1 atm and ν_{ki} is the stoichiometric coefficients

TNL Chemical Kinetics - II



The equilibrium constants

$$K_{pi} = \exp\left(\frac{\Delta S_i^o}{R} - \frac{\Delta H_i^o}{RT}\right)$$

The difference of forward rates (k_{fi}) and the reverse rates (k_{ri}) of reversible reaction generates the progress variable Q_i for the i^{th} reaction;

$$Q_i = k_{fi} \prod_{k=1}^{K} [X_k]^{\nu'_{ki}} - k_{ri} \prod_{k=1}^{K} [X_k]^{\nu''_{ki}}$$

$[X_k]$ is the molar concentration of species, ν_{ki} is the stoichiometric coefficients.

Deposition Process

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 $D_0 = \frac{2k_B T}{h}$

KINETIC MONTE CARLO (KMC)



- Surface activation energy is crucial factor to determine that bonds are formed solely between adjacent atoms.
- The different material systems have different surface activation energy of the atoms.
- Consequently, the overall surface activation energy is influenced by the surface diffusion energy barrier, the nearest neighbors binding energy, and the number of nearest neighbors (nn) present on the surface

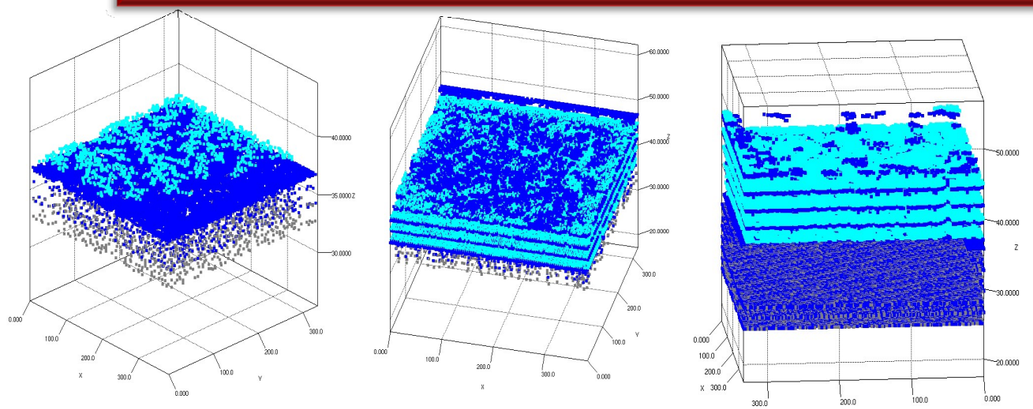
$$E = E_s \pm nE_n$$

Influence of step-edge barriers

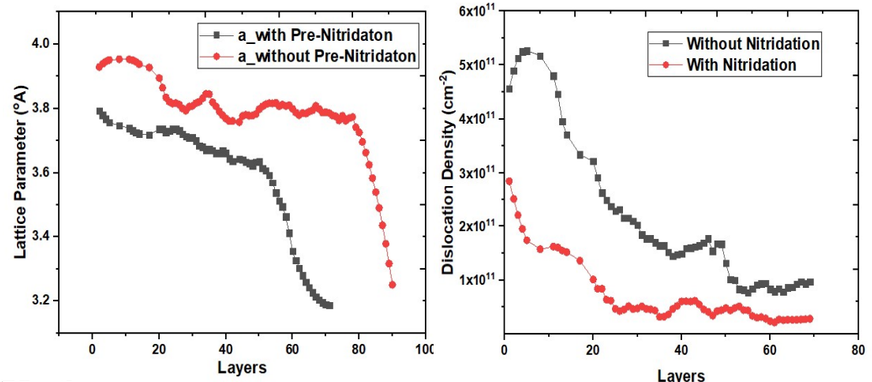
$$E = \begin{cases} E_s + nE_n + E_{shw} \\ E_s + nE_n + E_i \end{cases}$$

E_{shw} and E_i denote the Schwoebel and incorporation barriers energies respectively. These two barriers are destination dependent, so the activation energy for the same atom is also dependent on diffusion destination.

MOCVD Growth

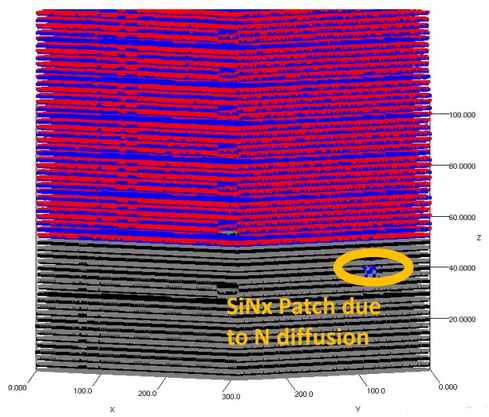


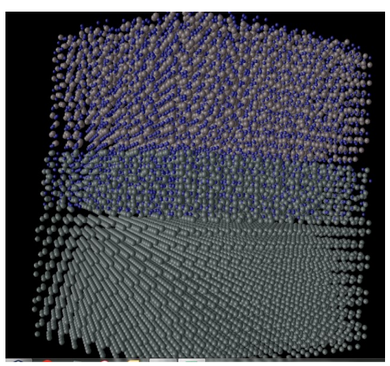
AlN on Si(111) with an NH3 pre-flow duration of 0, 5 and 30 seconds, 1, 4ML, 4ML-AlN extracted



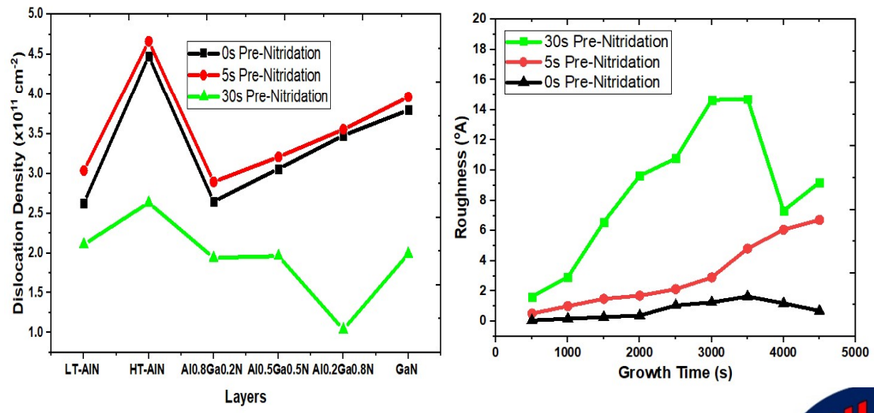
AlN/Si growth rates are well matched with Exp

Journal of Crystal Growth 630 (2024) 127584





Pre-Nitridation for 30 s



Influence of nitridation on the dislocation density at atomistic scale ,*Scientific Reports*, (12 April 2025) 15:12630

PALE Approach



PALE AlN Layer

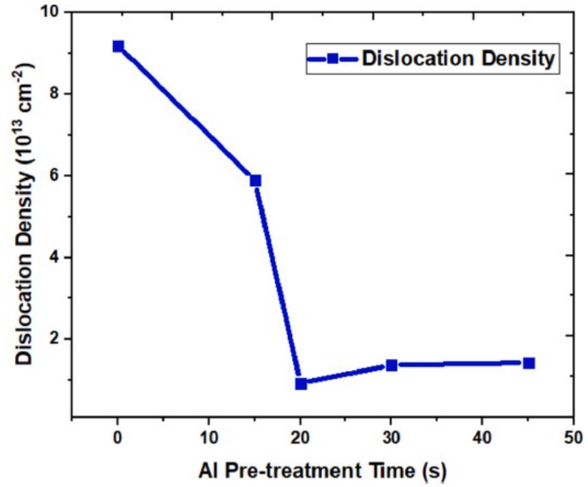
AlN Nucleation Layer

Si Substrate

PALE AlN Layer (1 loop)

	4 sec on	2 sec off
TMAl		
NH3	4 sec off	2 sec on

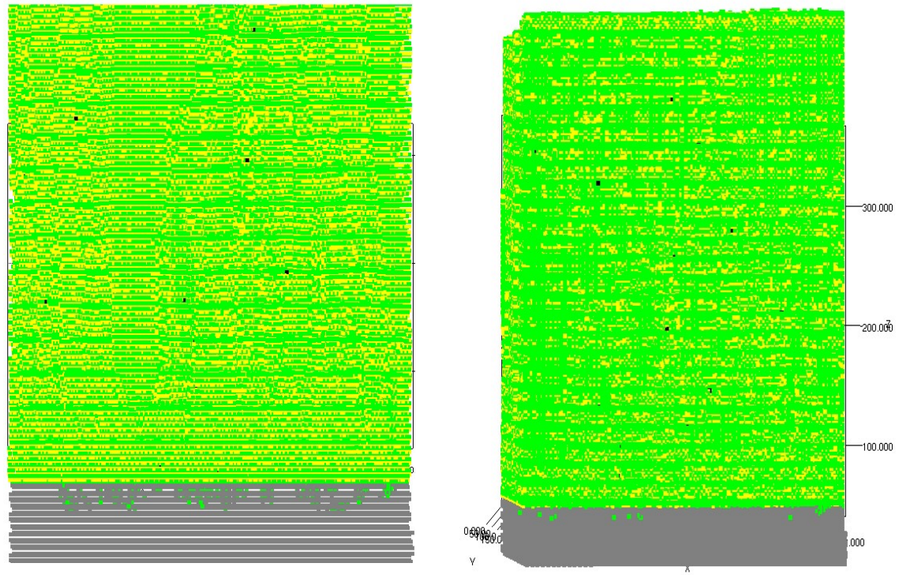
Parameters		Values
Lattice Parameters (A)	a	3.27522
	b	3.23405
	c	4.72923
Dislocation density		1.49E+11
% Vacancy		4.1%



Dislocation Density: variations in samples with TMAl pre-flow times of 0, 15, 20, and 45s.

Intrinsic carbon doping in GaN layers

Parameters		A	Exp	B	Exp	C	Exp
Growth Rate (nm/s)		0.7 ~ 0.9	~0.7*	0.23 ~ 1.5	0.2 ~ 1.3*	0.3 ~ 0.7	~ 0.7*
Lattice Parameters (^oA)	a	3.16	-	3.17	-	3.17	-
	b	3.16	-	3.17	-	3.17	-
	c	5.19	-	5.18	-	5.23	-
C_{avg} (cm^{-3})		~10^{17}	~10^{18}*	~10^{17}	~10^{18}*	~10^{17}-10^{18}	~10^{18}*
Dislocations (cm^{-2})		2.7x10^{11}	-	2.6x10^{11}	-	2.0x10^{11}	-

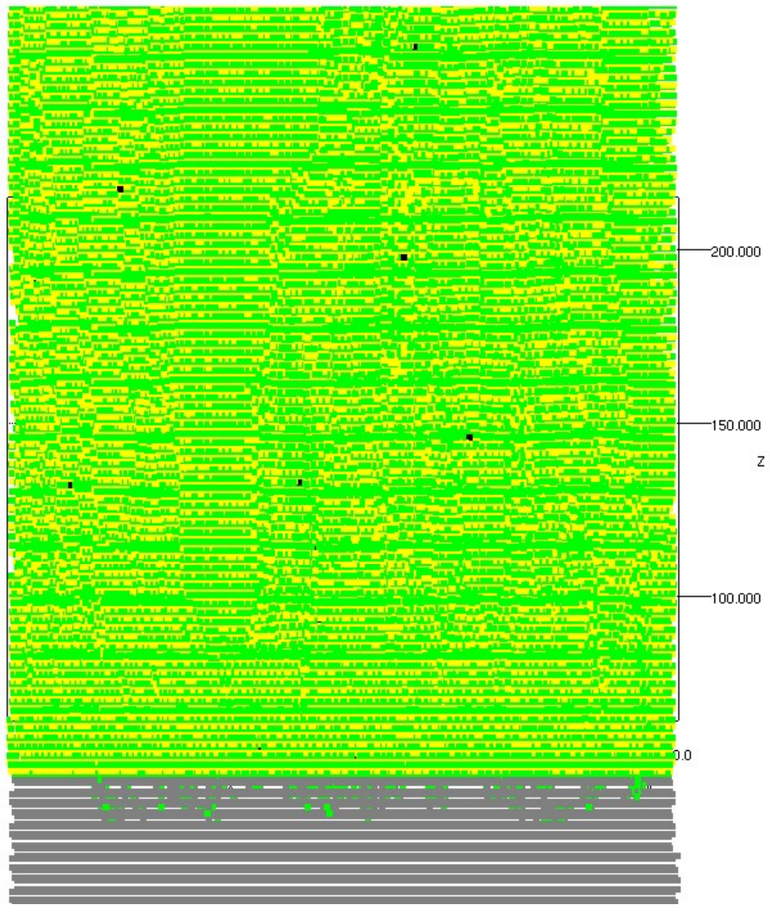


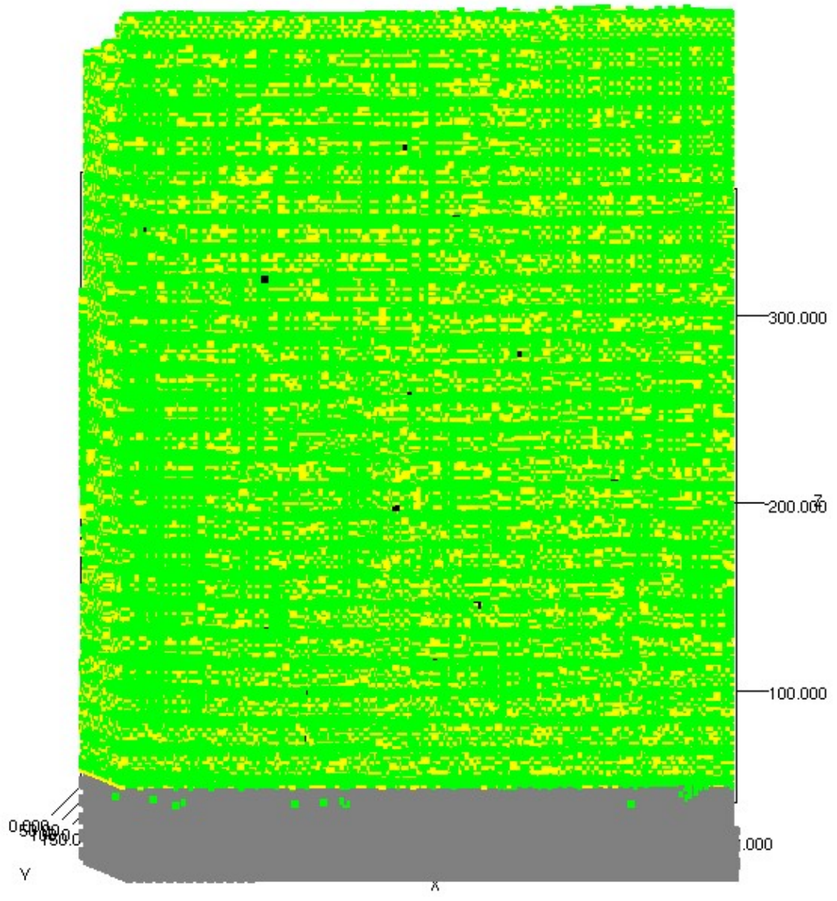
Substrate Size: 100 unit cell x 100 unit cell = 944.33 nm²

1 unit cell x 1 unit cell = 3.073 x 3.073 $^oA^2$ = 9.4433 $^oA^2$

Reactor geometry parameters from our partner are used

TRACES OF C IN SiC

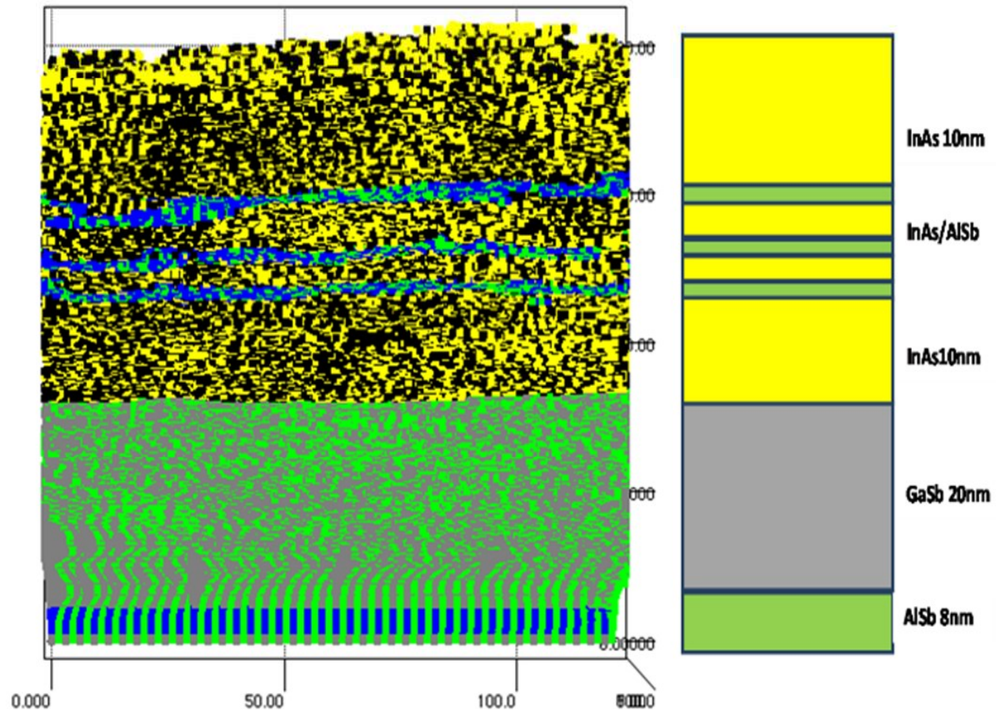




QUANTUM WELL

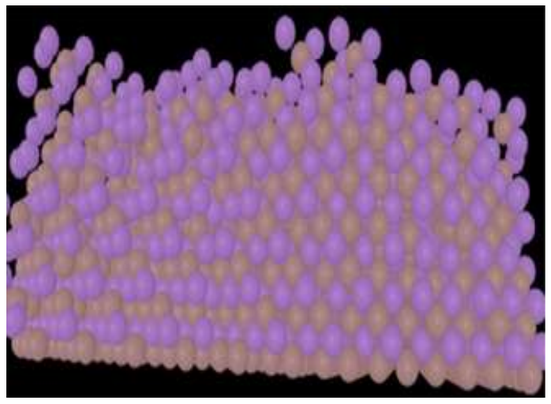


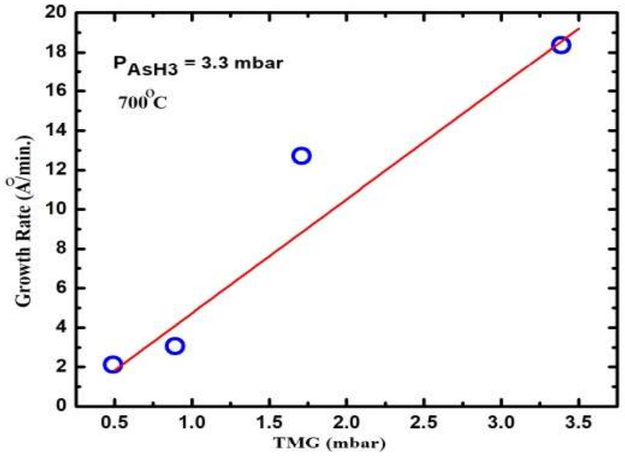
Layers	Lattice Parameters (A)			Vacancy (per A^{-3})	Dislocation (per A^{-2})
	a (A)	b (A)	c (A)		
AlSb	6.114	6.099	9.193	$1.1x10^{-5}$	0
GaSb	5.512	5.952	6.95	$3.2x10^{-3}$	$1.63x10^{-3}$
InAs	4.484	4.736	7.655	$5.4x10^{-3}$	$1.65x10^{-3}$
AlSb	4.194	4.191	7.81	$8.8x10^{-3}$	$1.25x10^{-3}$
InAs	4.286	5.564	7.253	$9.3x10^{-3}$	$1.27x10^{-3}$
AlSb	4.309	5.693	7.221	$6.4x10^{-3}$	$9.64x10^{-4}$
InAs	4.25	4.343	7.959	$7.3x10^{-3}$	$1.07x10^{-3}$
AlSb	4.201	4.312	7.63	$6.1x10^{-3}$	$7.26x10^{-4}$
InAs	4.018	4.236	7.827	$7.2x10^{-3}$	$1.03x10^{-3}$

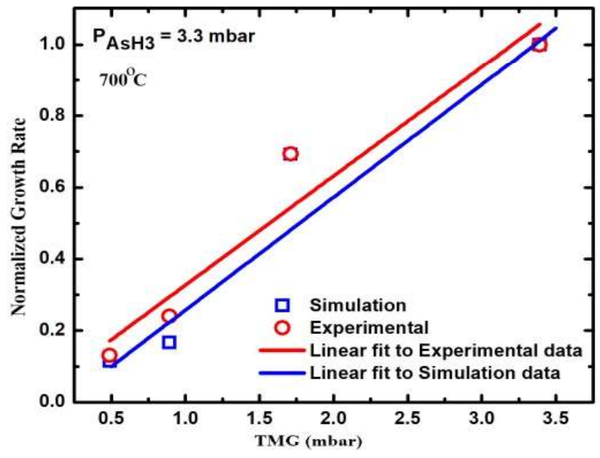


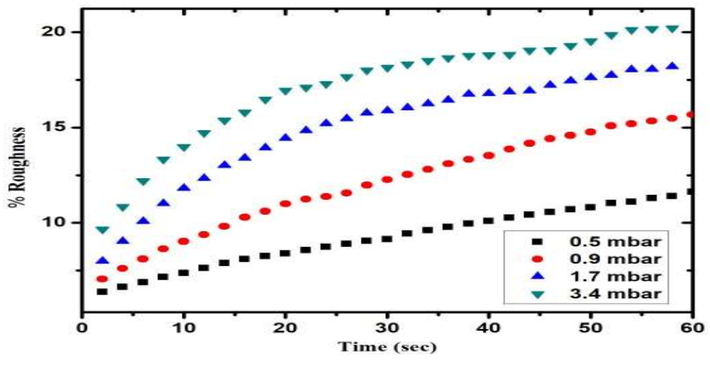
GaAs: MOCVD Showerhead

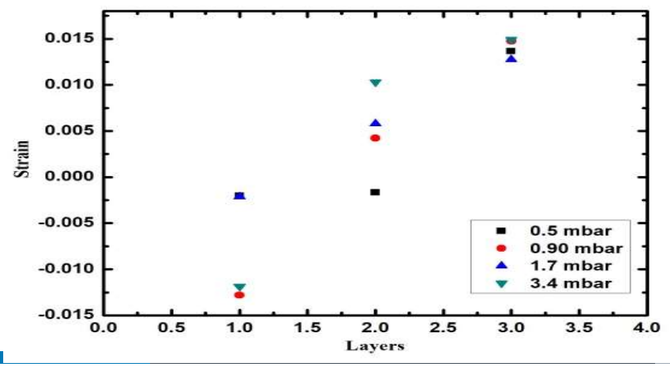








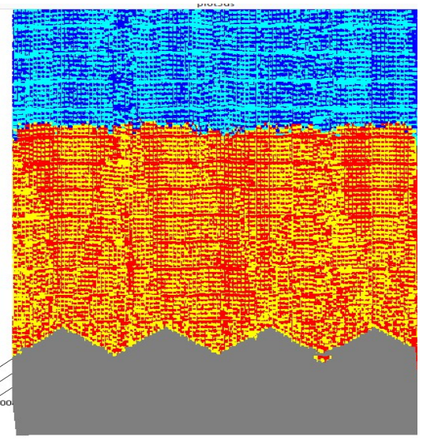


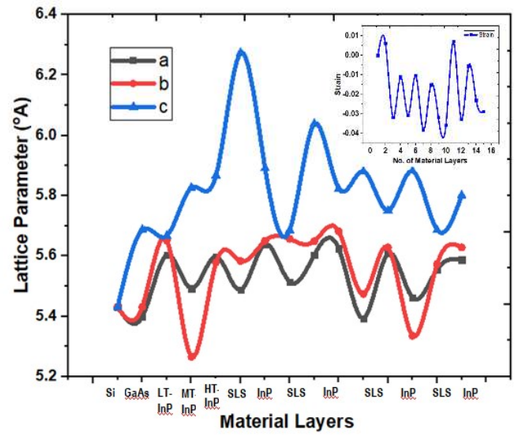


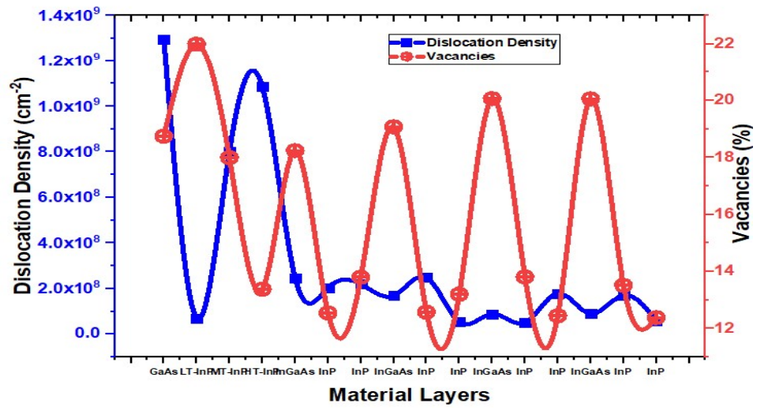
* Journal of Alloys and Compounds 809 (2019) 151752.

As & P: MOCVD Epitaxy

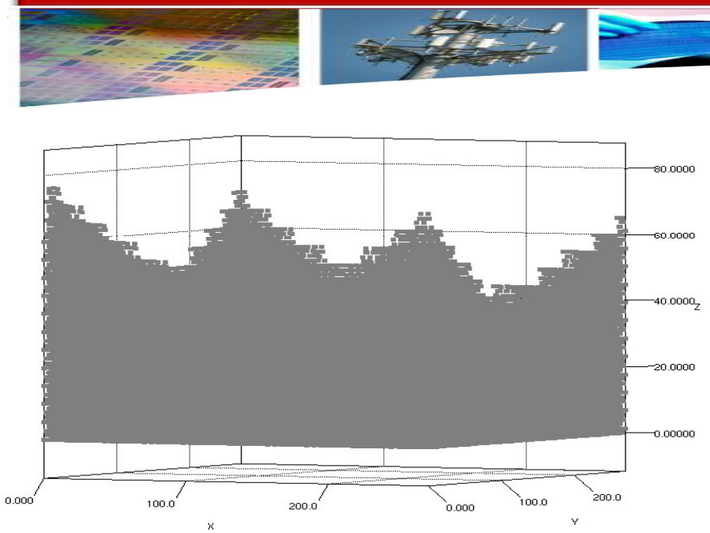
Material Layer		Growth Rate (A/sec)	Lattice Parameter (A) a	b	c	Strain	Dislocation (cm^{-2})	Point Defects %
2.0 µm GaAs over V-groove patterned (001) Si		1.468	5.5021	5.435	5.8944	-0.0131	2.76E9	19.54
LT-InP		0.9888	5.6501	5.6163	5.8557	-0.0403	3.13E8	23.31
MT-InP		3.1151	5.6374	5.332	5.8402	-0.038	3.58E8	17.53
HT-InP		4.0299	5.6092	5.5655	5.8787	-0.0328	3.49E8	12.7
InGaAs	10 Periods	0.853	5.652	5.682	5.7922	-0.0406	2.92E7	17.78
InP		3.8349	5.6594	5.6655	5.8214	-0.042	3.77E7	15.39
HT-InP spacer		4.05	5.6778	5.688	5.8755	-0.0454	5.80E7	13.83
InGaAs	10 Periods	0.8539	5.6515	5.6793	5.887	-0.0406	4.85E7	19.11
InP		3.8344	5.6664	5.6457	5.8303	-0.0433	7.71E7	17.03
HT-InP spacer		3.8438	5.6751	5.6452	5.7929	-0.0449	6.96E7	15.92
InGaAs	10 Periods	0.8355	5.6207	5.677	5.9952	-0.0349	8.77E7	18.23
InP		3.8287	5.5649	5.5952	5.8914	-0.0246	2.81E8	15.48
HT-InP spacer		4.06	5.6429	5.6369	6.0343	-0.039	6.00E7	12.38



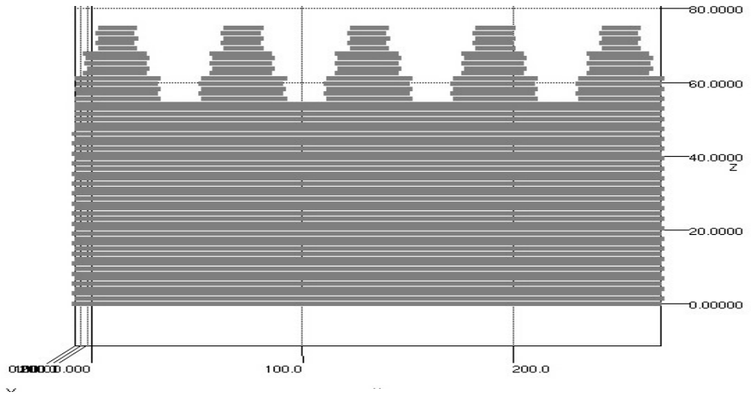


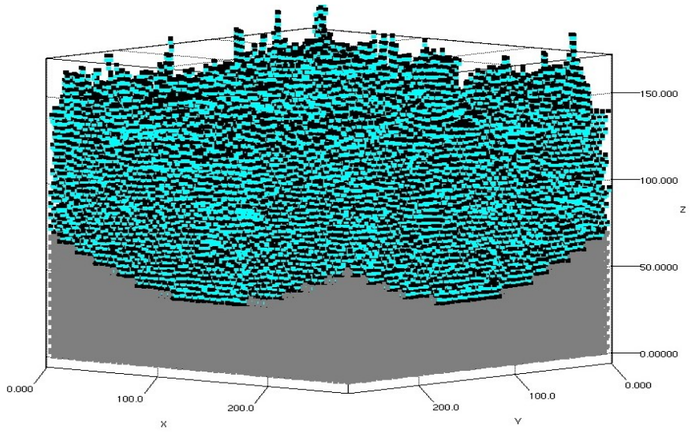


Patterned Substrate Epitaxy

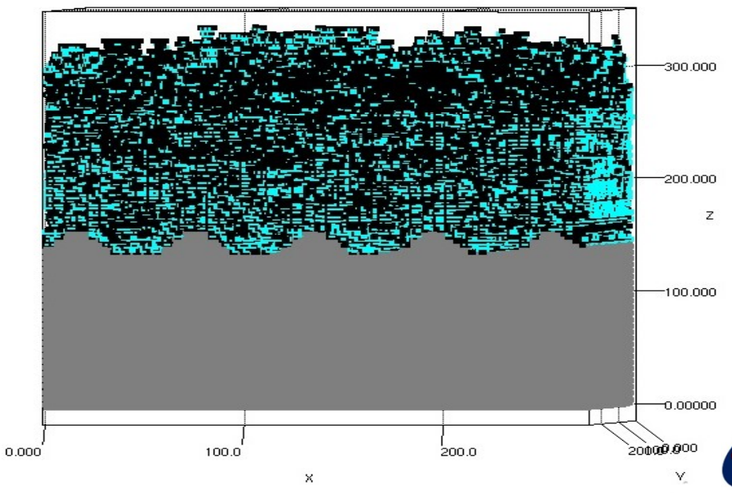


Substrate



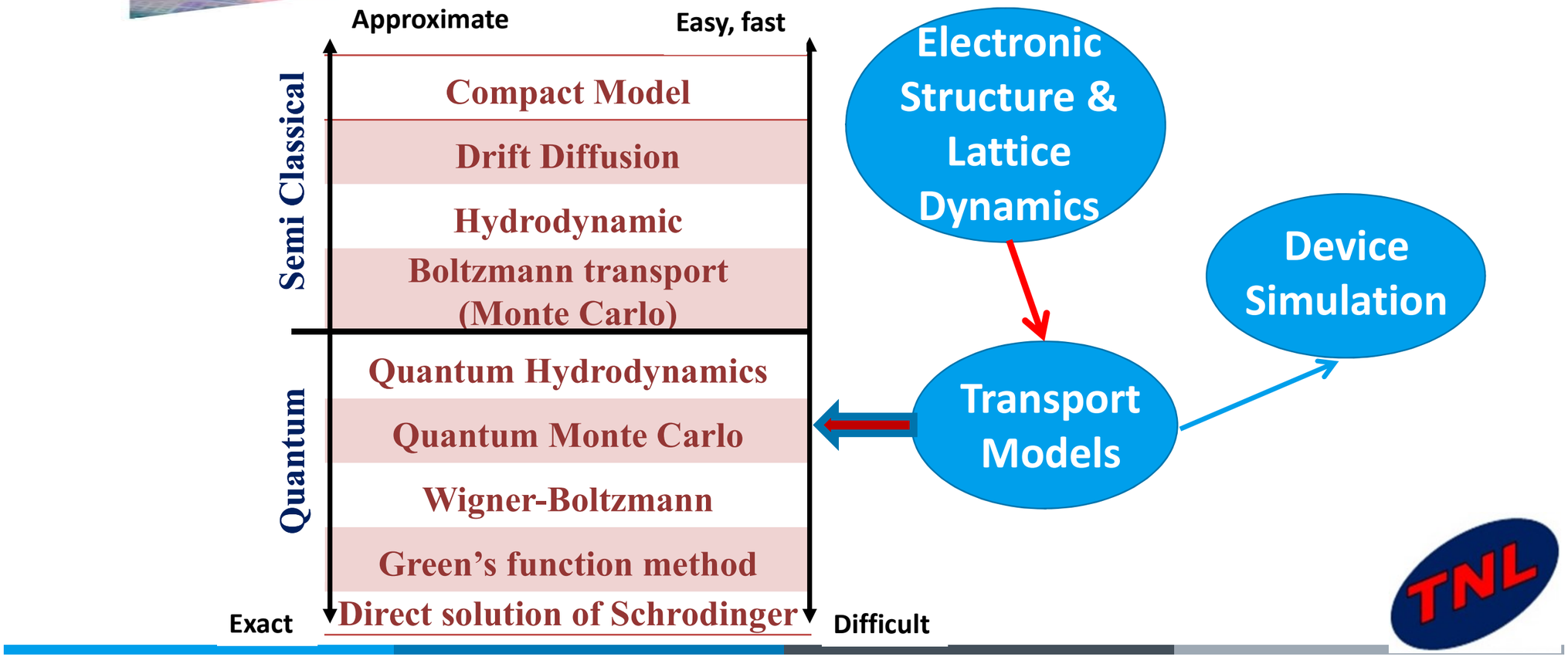


Epitaxy



Device Modeling





SOLUTION



- Transport of Monte Carlo particles (Super particles)
- Self-consistent solution of decoupled Poisson's and BTE equation over a small time-step
- The time step typically less than inverse plasma frequency
- Technologies implemented in Particle Device Simulator:
  - **MOSFET**
  - **FDSOI**
  - **Tunneling FET**
  - **MESFET**
  - **HEMT**
  - **GAA**
  - **FinFET**

- The classification of Particle-mesh (PM) coupling scheme is included as;
  - Carrier charge assign at mesh nodes through CIC, NGP, NEC schemes
  - Solution of Poisson's equation on node points through Successive over Relaxation (SOR) method,
  - Calculation of the mesh defined electric field components,
  - Interpolation of forces at the particle positions.

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Publications



- Angstrom-scale precision MOCVD epitaxy simulation for defect engineering and reproduction of high quality InP epitaxy on V-groove Si, **Materials Science in Semiconductor Processing** (2026) (Under Review)
- Uncovering GeO2 Epitaxy, , ***J. Vacc. Sci. Technology*** (2026) (Under Review)
- Family of 6.1 Semiconductor Epitaxy Solution, ***Journal of Crystal Growth*** 668 (2025) 128295 .
- Pre-Nitridation and its impact on dislocation density: III-N Epitaxy, ***Scientific Reports*** 15 (2025) 12630.
- Pre-Aluminization & Strain Analysis III-N Epitaxy, ***Journal of Crystal Growth*** 650 (2025) 127975.
- Full Electronic BandStructure Characterization: Al-Doped ZnO Nanocrystalline Films ***J. Elect. Mater.*** 53 (2024) 5885.
- Defect Analysis of HgCdTe Epitaxy on Si, GaAs, GaSb, and CZT Substrates, ***J. Electron. Mater.*** 53 (2024) 5803–5812.
- AlN MOCVD Epitaxy, ***Journal of Crystal Growth*** 630 (2024) 127584.
- Si and SiGe CVD Epitaxy, ***Materials Advances*** **5** (2024) 2110.
- Hot Carrier Dynamics in Ge, ***Sci. Rep.*** **13** (2023) 5630.
- ZnO nanofilm Characterization**, *J. Electron. Mater.*** **50(4)** (2021) 2417.
- Carrier Field Mobility of III-Nitrides, ***Sci. Rep.*** **10**, 18706 (2020).
- InGaAs based Photodetector. ***Optical and Quantum Electronics*** **52:**374 (2020).
- GaAs Epitaxy over GaAs*, **Journal of Alloys and Compounds*** **809**, 151752 (2019).
- Many more ……

Thank You

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