

To reduce the development cost, time and manpower consumption & to cater semiconductor material industry needs, TNL Epitaxial Material Growth CAD tools based on various reactor configurations will be useful and provide flexibilities to do hit & trail on computer with real reactor's geometries & various other input conditions.

Epi-Grow					– 🗆 X							
File Edit Simulate Help												
EpiGrow Run Output Epigrowth Input Conditions												
Upper Layer	Reactor (MOCVD)	MOCVD Precursor source			Substrate : Si Orientation : 100 Substrate Domain : 10.0 ¥ 10.0							
System ZincBle •	Steps 1	Chamber Condition	ShowerHead/Injector Para	motors	Substate Domain . 10.0 X 10.0							
Orientation 100	Time (Step 1) 5	Showerhead Based Injector Based	Shower hole's diameter	1.0								
Number of Layers	Time for Roughness		Chamber Volume (ltrs.) 1 Chamber Pressure 1	1.4 10 (torr 🔻								
Check Lattice Parameters	Temperature (C)		Ceiling Height (cm) 2 Chamber Temperature (C)	2.0								
Patterned Substrate	Surface Energy (ev) 2.0		Sticking Coeff.	1								
		Precurssor Condition										
Barrier Energies (eV)	No. of Interactive Elements	Number of Port	0 🛊									
Schwoebel 0.1	Atomic Number	Precursor 1	Select Prec									
Incorporation 0.1		Flow Rate	atm cc/s 💌	9,								
3.0	ADD	Load Reaction	Step 1	Load 1								
Add	Step 1 Reset											
					Go to Settings to activate Run we Exit							
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Features

- > TNL TCAD Tools are Graphical User Interface (GUI) based
- > Accurate and fast kinetic Monte Carlo (kMC) algorithms for reactor based deposition
- > No Statistical/thermodynamically assumptions or no use of any continuum models.
- > Chemical kinetics database available for gas- & surface phase reactions
- kMC technique controls random selection among three basic processes i.e. Adsorption, Diffusion or hopping and Desorption
- Various energy barriers E.g. Schwoebel–Ehrlich, incorporation and nearest neighbor etc barriers.
- > Chemical Reaction Kinetics; $\mathbf{k} = \mathbf{AT}^{n} \exp\left(-\frac{E_{a}}{\mathbf{p}_{T}}\right)$





Driven by Innovation

TECH NEXT LAB

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🔹 Reaction 🗕 🗆										□ ×			
TNL_Chemical Kinetics Precursors													
H2,SiH4				Output_Window									
No	No. Name		A n E(C			No.	Gas_Reaction	A	n	E(Cal)			
1 2 3 4 5 6	G 1 SiH4> SiH2 + H2 G 2 SiH4 + SiH2> Si2H6 G 3 Si2H6 + SiH2> HSISIH3 + G 4 Si2H6> H2 + HSISIH3 G 5 HSISIH3> H2 SISIH2 G 6 HSISIH3+H2> SIH2 + SIH4	9.49 10.26 14.24 9.96 13.40 13.97	1.7 1.7 0.4 1.8 0.2 0	54710 50200 8900 54200 5380 4092	Add_Gas)	1 2 3 4 5	G 1 SiH4 -→ SiH2 + H2 G 2 SiH4 + SiH2 -→ Si2H6 G 3 Si2H6 + SiH2 -→ HSISiH3 + SiH4 G 4 Si2H6 -→ H2 + HSISiH3 G 5 HSISIH3> H2SISIH2	9.49 10.26 14.24 9.96 13.40	1.7 1.7 0.4 1.8 0.2	54710 50200 8900 54200 5380			
No 2 3	. Name S 2 SiH2 + sigma> Si+H2 S 3 H2 + 2sigma> 2H*	A 11.76 11.36	n 0.5 0.5	E(Cal) 0 17250		No. 2 3	Surface_Reaction S 2 SiH2 + sigma> Si+H2 S 3 H2 + 2sigma> 2H*	A 11.76 11.36	n 0.5 0.5	E(Cal) 0 17250			
					Add_Surface								
Editor													
Add_Gas Save Add_Surface Save										Apply			

Deposition

Rates of each event help in calculating total rates

 $\mathbf{R} = \mathbf{A} + \mathbf{H} + \mathbf{D}$

Here A, H and D are the adsorption, diffusion and desorption rates respectively.

Outputs

- Surface roughness
- Average & layer by layer Strain profiling
- Types Defects with location in the lattice
 - Vacancies (Point Defect)
 - Interstitials (Point Defect)
 - Dislocation (Line Defect)
 - o Impurities in the lattice
 - Stacking faults
- Lattice parameter
- Growth rate with mole fraction



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CVD Reactor Process



- Currently laminar CVD reactor architecture is implemented with two types of separate operations including gases/vapors precursors and a chunk of volatile material can be used inside the chamber e.g. gallium etc as well.
- > The chamber temperature causes the precursor gases to react or decompose into the desired atoms/molecules and adsorb over the substrate surface.
- > Tube and precursors parameters like tube length, tube diameter, viscosity and other chamber conditions are required for initiating the CVD growth process.

Capabilities

- **o** Optimize Reactor based growth conditions
- Availability of various material database
- o Optimize chemical kinetics i.e. probabilities of various chemical reactions and reaction paths
- Predictive growth rates with mole fractions extraction
- Defects extraction qualitatively and quantitatively
- o Extraction of Strain: Average and within each monolayer
- Surface Profiling (Surface Roughness)
- Fewer experiments for optimization
- **o** Optimize reduction in waste during experimentation
- o Ability to deal with different reactive species and reactor geometries
- Explore rigorous physical information at Atomistic Scale
- On-line growth process control
- Cost effective solution: wafer and other growth industry



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MOCVD-Showerhead Reactor Process



Features

- Showerhead flange & inlets very close to substrate.
- Reactant gases are injected vertically from the showerhead flange
- > Reactant gases travel across the boundary layer onto the substrate surface by diffusion.
- Optimizing the space HC to suppress convection & gas residence time to use reactant gases efficiently
- Ld/R <1 convection, & Ld/H_c>1 diffusion
- Chemical kinetics database available for gas- & surface phase reactions
- > Residence time; $t_{res} = -\frac{H_c}{v_{in}} ln \frac{\delta}{H_c} + \frac{\delta^2}{4D}$

where δ is the boundary layer thickness in stagnation flow, Hc is the ceiling height, vin the inlet velocity and D is the mass diffusivity.



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MOCVD-Injector Reactor Process



Features

- Symmetry with AIXTRON AIX 200/4 horizontal MOCVD reactor
- Boundary conditions dependent film growth prediction ability
- > To develop new chemical kinetic path & reactions
- Optimize transport phenomena i.e. distribution of gas flow, temperature and species concentration in the reactor chamber
- > A complete reaction kinetics mechanism as well as a comprehensive transport phenomena modeling
- Diffusion behavior of each gas species in gas mixture depends on the temperature and pressure,

$$D_i = 2.7 \times 10^{-3} \frac{\sqrt{T^3 (M_i + M_{H_2})/(2 \times 10^3 M_i M_{H_2})}}{p \sigma_i \sigma_{H_2} \Omega_{\rm D}}$$

M is molecular weight (kg/mol), $\Omega_{
m D}$ is the collision integral and σ is the characteristic length (A°) of the Lennard–Jones potential.

- > Chemical kinetics database available for group III-V.
- > Descending steps in form of Schwoebel-Ehrlich barrier and ascending steps in form of incorporation barrier





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PECVD Reactor Process



Features

- > A single-wafer parallel electrode PECVD process with showerhead architecture
- > Characterization of the physico-chemical phenomena including glow discharge chemistry,
- Material to be coated amorphous silicon, SiO2, Si3N4 and SiC
- Impact of RF powers on plasma density in an Ar/O2 mixture
- Plasma use as a continuum medium,
- Physical properties of the gases assumed constant,
- Negligible volume change of the reacting gases,
- Azimuthal reactor geometry,



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Molecular Beam Epitaxy (MBE) Reactor Process



Features

- > MBE reactor can handle muktiple Effusion Cells at a time.
- > Vapour pressure of elements are calculated on the basis of known available database inbuilt.
- Chamber conditions as substrate to effusion cell distance, substrate temperature etc. are mandatory requirement.

