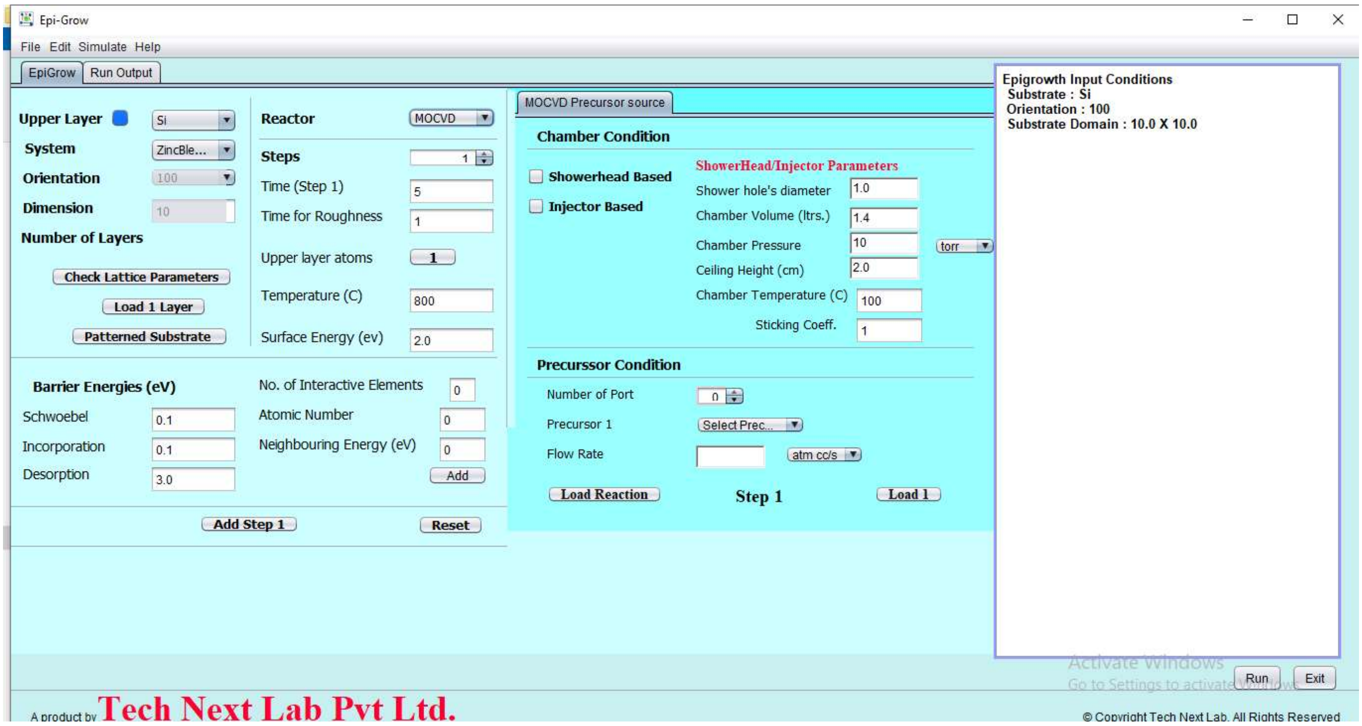
TECH NEXT LAB

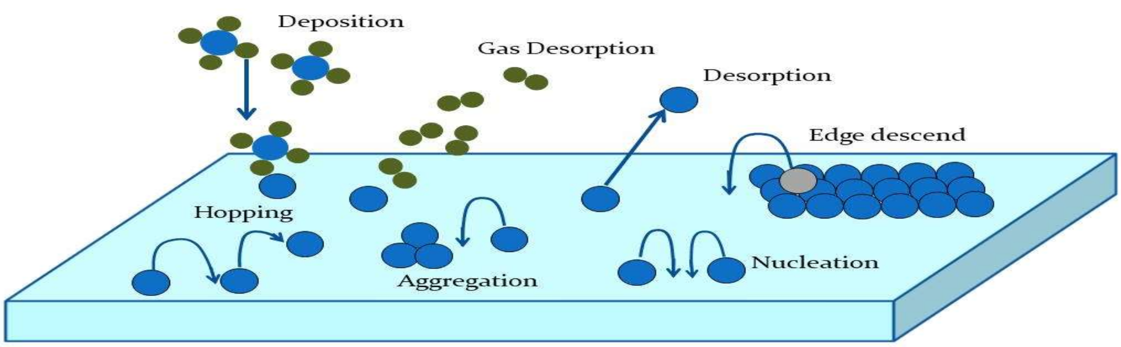
Technology of Next Level
Driven by Innovation

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.



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



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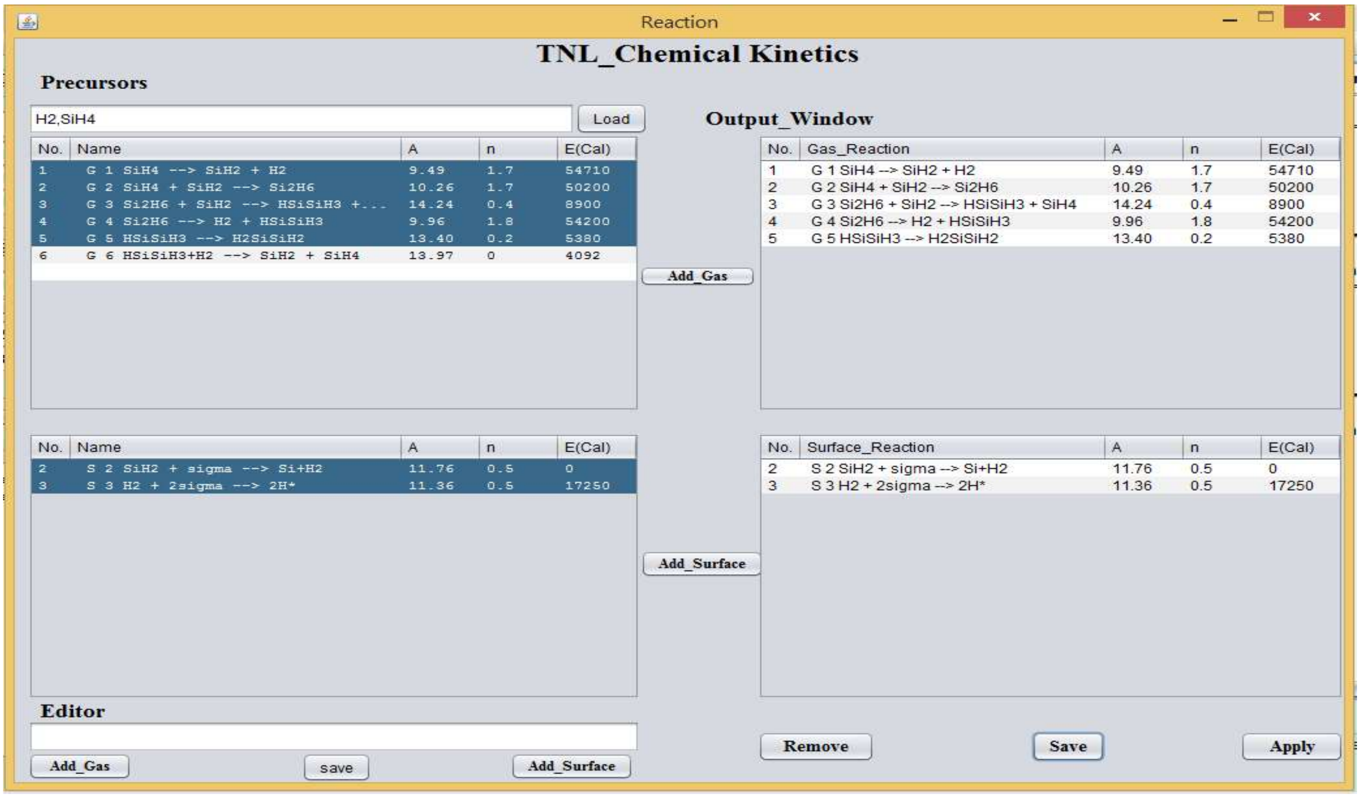

Deposition

❖ **Rates of each event help in calculating total rates**

$$R = A + H + D$$

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*)**
  - **Impurities in the lattice**
  - **Stacking faults**
- **Lattice parameter**
- **Growth rate with mole fraction**

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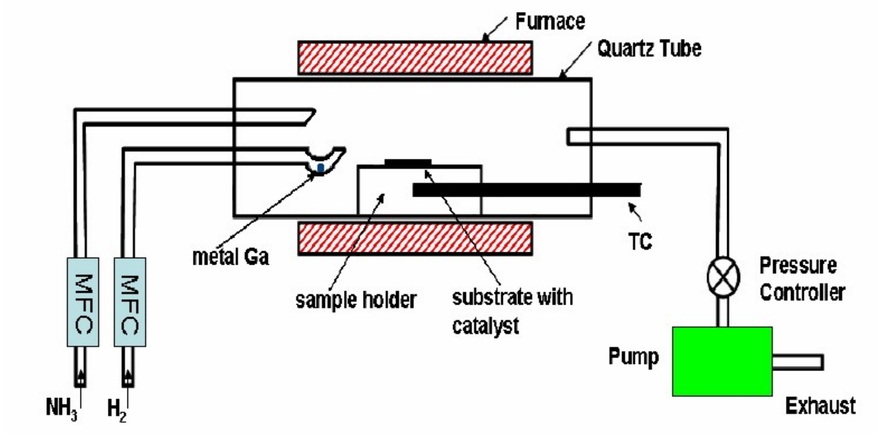
CVD Reactor Process



- **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

- **Optimize Reactor based growth conditions**
- **Availability of various material database**
- **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**
- **Extraction of Strain: Average and within each monolayer**
- **Surface Profiling (Surface Roughness)**
- **Fewer experiments for optimization**
- **Optimize reduction in waste during experimentation**
- **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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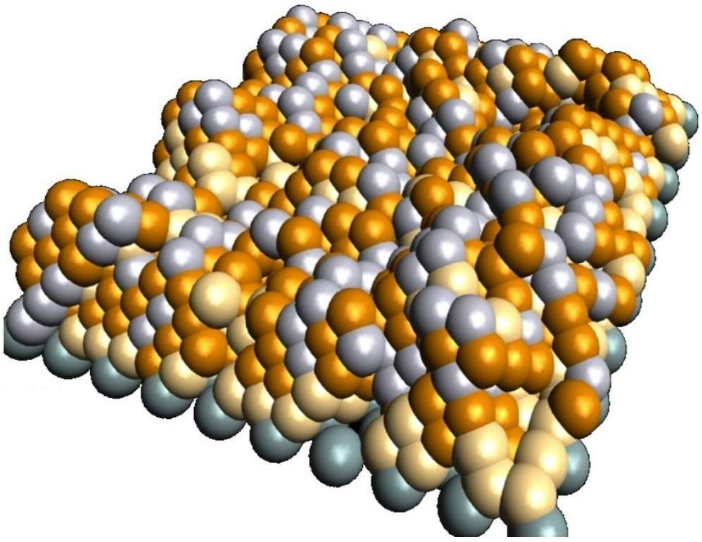

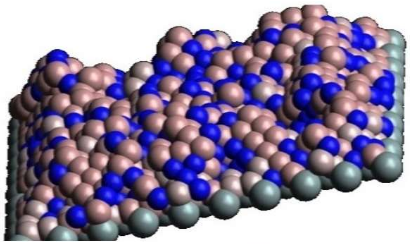

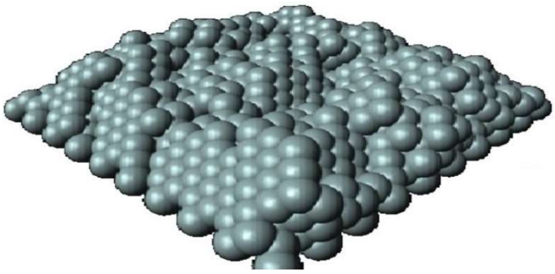

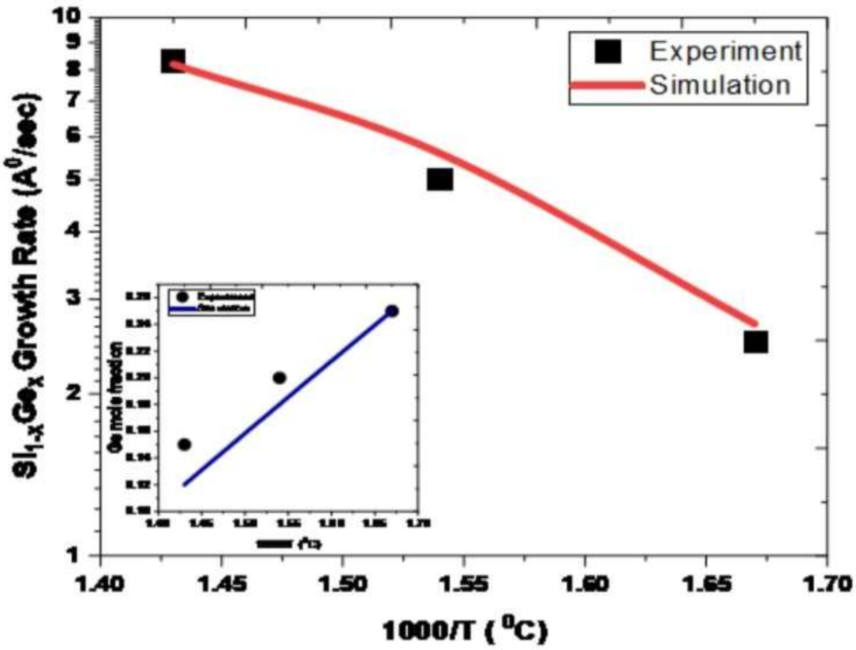

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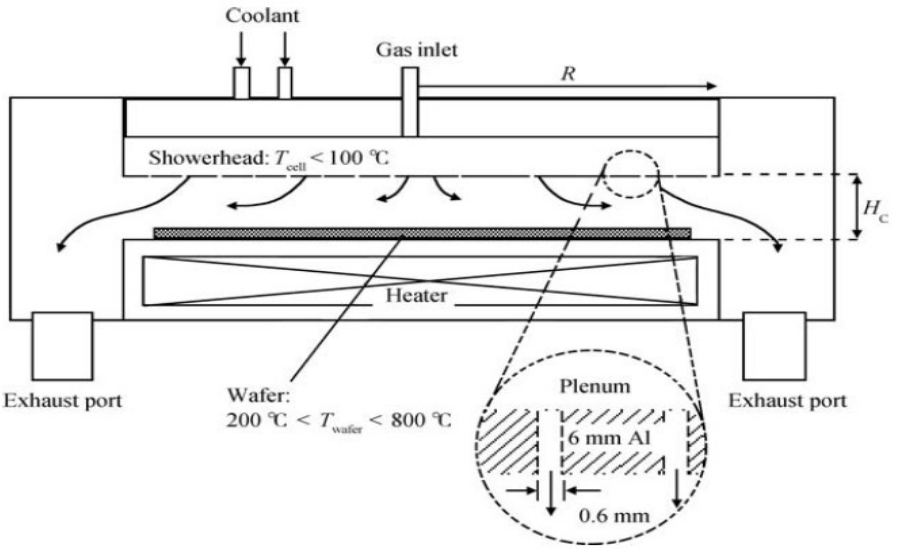
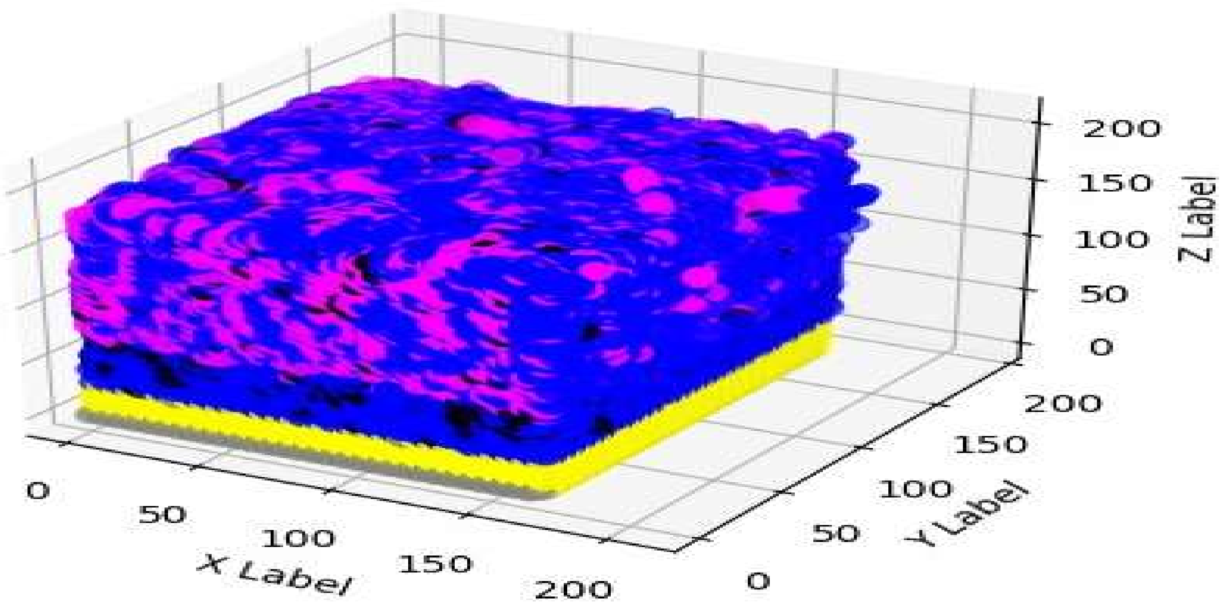
MOCVD-Showerhead Reactor Process



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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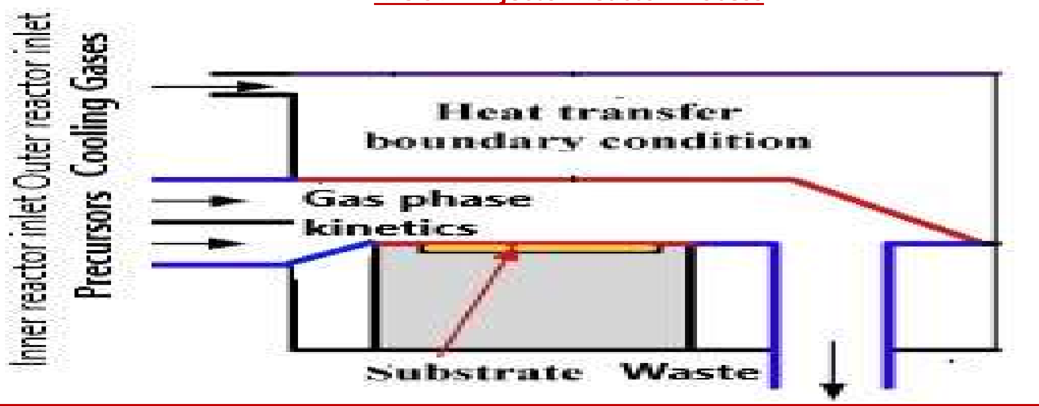
MOCVD-Injector Reactor Process



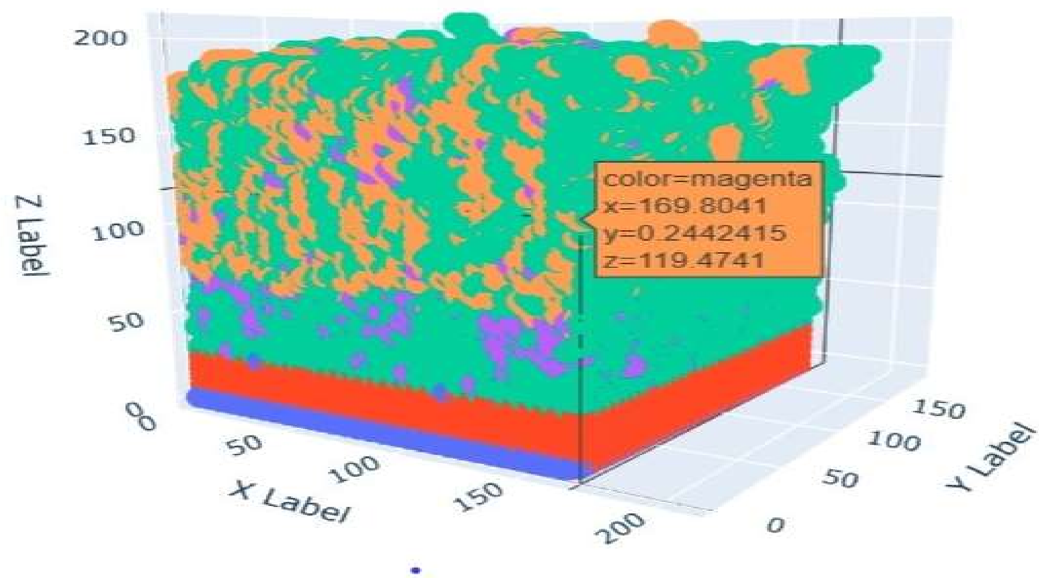
Features

- 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,

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

M is molecular weight (kg/mol), Ω_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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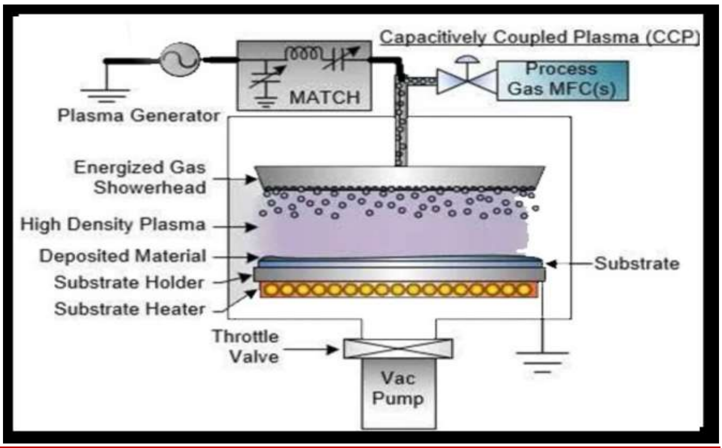
PECVD Reactor Process



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, SiO_2, Si_3N_4 and SiC
- Impact of RF powers on plasma density in an Ar/O_2 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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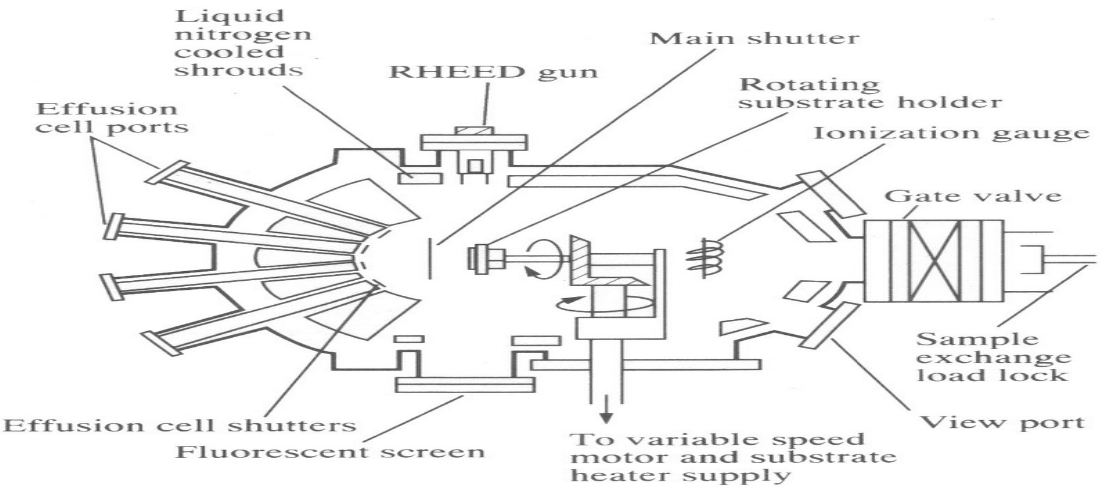
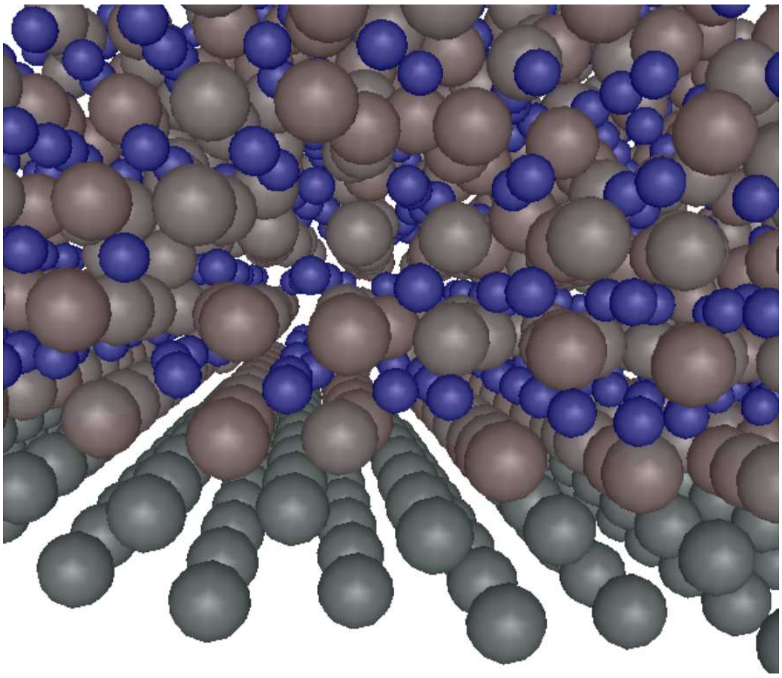
Molecular Beam Epitaxy (MBE) Reactor Process



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.**



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