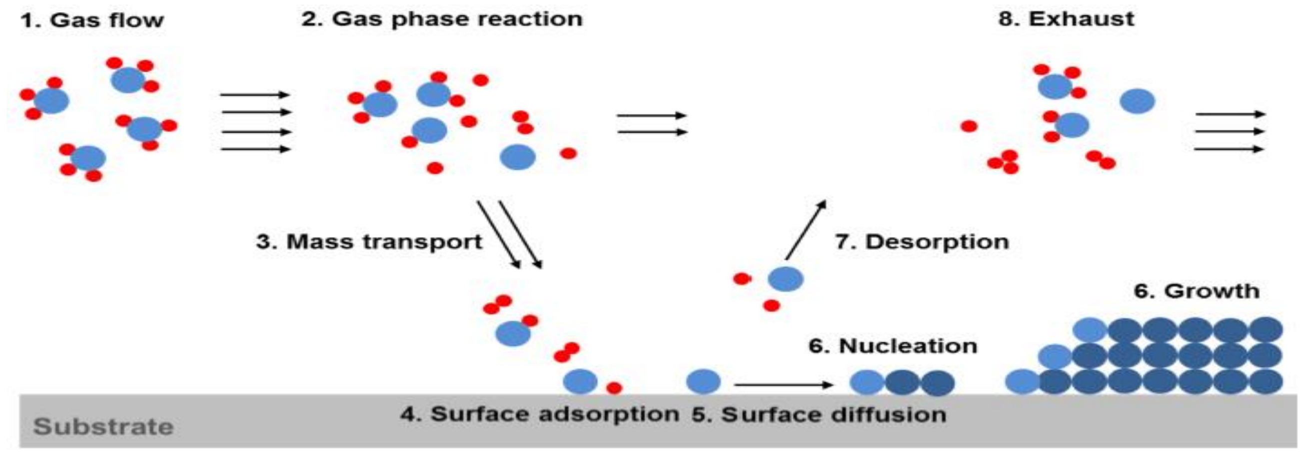
Atomistic Thin Film Growth – EpiGrow Simulator

Chemical Vapor Deposition (CVD)



Introduction

EpiGrow Simulator, CVD Reactor algorithms include Chemical vapor deposition is a process that involves the reaction of a volatile precursor which is injected into a chamber (typically under vacuum). The chamber is heated to a reaction temperature that causes the precursor gas to react or break down into the desired coating and bond to the material surface. Over time the coating material builds on the surface and creates a coating throughout the exposed part's surface.

Features

- In EpiGrow CVD Simulator having Stoichiometery i.e. exact composition of film
- Ultra-pure precursor gases are injected into a reactor, no possibility of contaminations.
- Conformality and step coverage

T N L

- Laminar fluid flow" i.e., smooth flow with no turbulence
- Transport flux of reactant through the boundary layer

Physics

1. Fluid Flow equations used:

Assuming "laminar flow" i.e., smooth flow with no turbulence. Force F on the fluid is defined as:

$$F = \mu \frac{dv}{dz}$$

Here,

v = velocity of fluid, z = distance from the surface, μ= viscosity of fluid

2. Fluid flow is often measured by Reynolds number Re.

$$Re = \frac{dv\rho}{\mu}$$

Here,

d = length of system (diameter of pipe), ρ = density of fluid, v = velocity

3. Laminar Boundary thickness varies as distance from flow start

$$\delta = \frac{l}{\sqrt{Re}}$$

Here,

Re = Reynolds number, l = distance from the substrate

4. Transport flux of reactant through the boundary layer

$$j = \frac{D}{\delta}\left(N_g - N_0\right)$$

Here,

D = the diffusion coefficient, Ng = concentration at top of boundary layer, N_0 = concentration at surface

5. Diffusion Coefficient is given as

$$D \propto T^{\frac{3}{2}} \frac{Ps}{P}$$

Here,

T = Temperature (K), Ps = partial pressure of diffusing species, P = total pressure

T N L

Reaction at Substrate Surface

1. **Flux at surface controlled by reaction**

$$J = K_s N_g$$

Here,

Ks = surface reaction rate, Ng = concentration at top of boundary layer

2. **Reaction rate flows an Arrhenius law**

$$K_s = k' exp\left(\frac{-Ea}{RT}\right)$$

Here

k' = reaction constant, Ea = Activation energy of the reaction, RT = thermal energy (eV)

3. **The Reaction Flux at the surface**

$$J = \frac{DKs\,Ng}{D + \delta Ks}$$

4. **Thus the reaction rate of CVD process is given by**

$$r = \frac{J}{\gamma} = \frac{DKs\,Ng}{\gamma(D + \delta Ks)}$$

Benefits can be realized

- **Graphical User Interface (GUI) based Simulator**
- **Binary, ternary and quaternary compound semiconductor based epitaxial growth**
- **Users have flexibilities to accommodate by inputting their own chemical reactions as text file**
- **Surface profiles Extracting Roughness**
- **Defects Extraction (point/clusters)**
- **Extraction of dislocations & Stress/Strain**
- **Fewer experiments for optimization**
- **Reduction in waste during experimentation**
- **Ability to deal with different reactive species and reactor geometries**
- **On-line process control**