

Given Problem:-

For Physical Vapor Deposition:-

Assumptions:-

- 1D growth:- Crystal grows only in the x direction from $x=0$ to $x=L(t)$.
- Instantaneous crystallization:- every molecule arriving at the interface adheres with 100% efficiency.
- Isothermal interface:- Interface temperature $T_{int}(t)$ is prescribed.
- Constant properties
- Negligible vapor-side resistance: mass flux $J_m(t)$ is taken as known (or shaped into an empirical growth rate).

Governing Equations:-

- Heat conduction of the solid:-

$$\rho_s c_s \frac{\partial T}{\partial t} = k_s \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < L(t)$$

- Stefan (energy) condition at $x = L(t)$

$$\rho_s \Delta H \frac{dL}{dt} = -k_s \left. \frac{\partial T}{\partial x} \right|_{x=L(t)}$$

- Kinematic growth law:-

$$\rho_s \frac{dL}{dt} = J_n(t) M$$

Boundary & initial conditions:-

- At the seed $z=0$:- $T(g, t) = T_{seed}$

- At the interface $z=L(t)$:-

$$T(L(t), t) = T_{int}(t)$$

- Initial state at $t=0$:-

$$L(0) = L_0, \quad T(g, 0) = T_{init}(t)$$

Chemical Vapor Deposition:-

Assumption:-

- 1) 1D Boundary Layer:- gas-phase concentration varies only in $0 < z < \delta$
- 2) Steady gas flow:- velocity is constant, convection
- 3) First-order surface reaction:- deposition flux proportional to surface concentration
- 4) Instantaneous incorporation:- every adsorbed molecule becomes solid.
- 5) Constant properties:- $\rho_s, c_s, k_s, \Delta H, D, \mu, k_{chem}$ constant.

Governing equations:-

- Gas-phase convection-diffusion ($0 < x < \delta$)

$$u \frac{\partial c_g}{\partial x} = D_g \frac{\partial^2 c_g}{\partial x^2}$$

- Surface reaction flux at $x=0$:-

$$J_{surf}(t) = k_{chem} c_g(t)$$

- Film heat conduction:-

$$\rho_s k_s \frac{\partial T}{\partial t} = k_s \frac{\partial^2 T}{\partial x^2}$$

- Energy (Stefan) balance at the growing surface $x=0$:-

$$\rho_s \delta H \frac{dL}{dt} = -k_s \frac{\partial T}{\partial x} \Big|_{x=0}$$

- Kinematic growth law:-

$$\rho_s \frac{dL}{dt} = J_{surf}(t) M_{film}$$

Boundary and initial conditions:-

Gas layer:- $c_g(\delta, t) = c_\infty$

Film temperature:-

$$T(L(t), t) = T_{sub} - k_s T_x(0, t) = J_T [T(0, t) - T_\infty]$$

Initial state at $t=0$:-

$$L(0) = 0; T(x, 0) = T_{init}(x), c_g(x, 0) = c_\infty$$