**Mathematical Model for Semiconductor Recipe Optimization**

**1. Thermal Dynamics Model**

**1.1 Heat Conduction in Wafer**

The temperature distribution in the wafer follows the heat equation:

∂T/∂t = α∇²T + Q(x,y,z,t)/ρc\_p

Where:

* T(x,y,z,t): Temperature distribution
* α: Thermal diffusivity
* Q(x,y,z,t): Heat source term (from plasma, lamps, etc.)
* ρ: Density
* c\_p: Specific heat capacity

**1.2 Boundary Conditions**

* Surface heat flux: q = h(T\_surface - T\_ambient)
* Radiative heat transfer: q\_rad = εσ(T⁴ - T\_amb⁴)

**2. Chemical Vapor Deposition (CVD) Model**

**2.1 Gas-Phase Transport**

Species continuity equation:

∂C\_i/∂t + ∇·(C\_i v) = D\_i∇²C\_i + R\_i

Where:

* C\_i: Concentration of species i
* v: Velocity field
* D\_i: Diffusion coefficient
* R\_i: Reaction rate

**2.2 Surface Reactions**

For precursor adsorption and deposition:

∂θ\_i/∂t = k\_ads C\_i(1-θ\_total) - k\_des θ\_i - k\_react θ\_i

Where:

* θ\_i: Surface coverage fraction
* k\_ads, k\_des, k\_react: Rate constants

**2.3 Film Growth Rate**

dh/dt = (M\_film/ρ\_film) Σ(ν\_i R\_i)

Where:

* h: Film thickness
* M\_film: Molecular weight
* ν\_i: Stoichiometric coefficient

**3. Plasma Etching Model**

**3.1 Plasma Chemistry**

Ion density evolution:

∂n\_i/∂t = ∇·(D\_i∇n\_i) - μ\_i∇·(n\_i E) + S\_i - L\_i

Where:

* n\_i: Ion density
* μ\_i: Mobility
* E: Electric field
* S\_i: Source term
* L\_i: Loss term

**3.2 Etch Rate Model**

R\_etch = (Y\_phys + Y\_chem) Γ\_ion

Where:

* Y\_phys: Physical sputtering yield
* Y\_chem: Chemical enhancement factor
* Γ\_ion: Ion flux

**3.3 Profile Evolution**

Level set method for etch front:

∂φ/∂t + R\_etch|∇φ| = 0

**4. Dopant Diffusion Model**

**4.1 Diffusion Equation**

∂C/∂t = ∇·(D\_eff∇C) + G - R

Where:

* C: Dopant concentration
* D\_eff: Effective diffusion coefficient
* G: Generation term
* R: Recombination term

**4.2 Concentration-Dependent Diffusivity**

D\_eff = D\_0 + D\_E(C/C\_ref)^n

**5. Stress and Deformation Model**

**5.1 Mechanical Equilibrium**

∇·σ + f = 0

Where σ is the stress tensor and f is body force.

**5.2 Thermal Stress**

σ\_thermal = E α\_thermal ΔT/(1-ν)

**5.3 Intrinsic Film Stress**

σ\_intrinsic = f(deposition\_rate, T, pressure)

**6. Electrical Characterization**

**6.1 Carrier Transport**

Drift-diffusion equations:

∂n/∂t = (1/q)∇·J\_n + G - R

∂p/∂t = -(1/q)∇·J\_p + G - R

Where:

* n, p: Electron and hole concentrations
* J\_n, J\_p: Current densities
* G, R: Generation and recombination rates

**6.2 Current Densities**

J\_n = qμ\_n n∇φ + qD\_n∇n

J\_p = qμ\_p p∇φ - qD\_p∇p

**7. Defect Formation Model**

**7.1 Point Defect Dynamics**

∂C\_V/∂t = ∇·(D\_V∇C\_V) + G\_V - R\_V

∂C\_I/∂t = ∇·(D\_I∇C\_I) + G\_I - R\_I

Where:

* C\_V, C\_I: Vacancy and interstitial concentrations
* G\_V, G\_I: Generation rates
* R\_V, R\_I: Recombination rates

**8. Process Parameter Dependencies**

**8.1 Temperature-Dependent Rate Constants**

k = k\_0 exp(-E\_a/kT)

**8.2 Pressure-Dependent Transport**

D\_eff = D\_0 (P\_0/P)^n

**8.3 Power-Dependent Plasma Parameters**

n\_e = n\_0 (P\_rf/P\_0)^α

T\_e = T\_0 (P\_rf/P\_0)^β

**9. Optimization Objective Function**

**9.1 Multi-Objective Function**

J = w\_1 J\_uniformity + w\_2 J\_rate + w\_3 J\_selectivity + w\_4 J\_defects

Where:

* J\_uniformity: Uniformity metric
* J\_rate: Process rate metric
* J\_selectivity: Selectivity metric
* J\_defects: Defect density metric

**9.2 Uniformity Metric**

J\_uniformity = (1/A)∫∫[(h(x,y) - h\_target)²]dxdy

**9.3 Rate Metric**

J\_rate = |R\_process - R\_target|/R\_target

**10. Constraints**

**10.1 Physical Constraints**

* Temperature limits: T\_min ≤ T ≤ T\_max
* Pressure limits: P\_min ≤ P ≤ P\_max
* Flow rate limits: F\_min ≤ F ≤ F\_max

**10.2 Process Constraints**

* Minimum film thickness: h ≥ h\_min
* Maximum etch rate: R\_etch ≤ R\_max
* Stress limits: |σ| ≤ σ\_yield

**11. Boundary and Initial Conditions**

**11.1 Thermal Boundaries**

* Wafer chuck: T = T\_chuck
* Top surface: Convection/radiation to ambient

**11.2 Mass Transport Boundaries**

* Inlet: C\_i = C\_inlet,i
* Outlet: ∇C\_i·n = 0
* Walls: Robin boundary conditions

**11.3 Initial Conditions**

* T(x,y,z,0) = T\_initial
* C\_i(x,y,z,0) = C\_initial,i
* h(x,y,0) = h\_initial

**12. PINN Implementation Considerations**

**12.1 Physics Loss Terms**

L\_physics = L\_PDE + L\_BC + L\_IC + L\_constraints

**12.2 Data Loss Terms**

L\_data = Σ|u\_pred - u\_measured|²

**12.3 Total Loss Function**

L\_total = λ\_phys L\_physics + λ\_data L\_data + λ\_reg L\_regularization

**13. Recipe Parameters for Optimization**

**13.1 Process Parameters**

* Temperature profile: T(t)
* Pressure: P(t)
* Gas flow rates: F\_i(t)
* RF power: P\_rf(t)
* Processing time: t\_process

**13.2 Material Parameters**

* Precursor concentrations
* Etchant concentrations
* Carrier gas compositions

**13.3 Equipment Parameters**

* Chamber geometry
* Electrode spacing
* Magnetic field strength

**14. Validation Metrics**

**14.1 Film Quality Metrics**

* Thickness uniformity: σ\_thickness/μ\_thickness
* Composition uniformity
* Crystalline quality (XRD)
* Surface roughness

**14.2 Electrical Metrics**

* Sheet resistance
* Mobility
* Carrier concentration
* Breakdown voltage

**14.3 Yield Metrics**

* Defect density
* Particle contamination
* Pattern fidelity
* Critical dimension control