7TH SEMATECH AEC AND APC WORKSHOP

Optimal Control for LPCVD Processes

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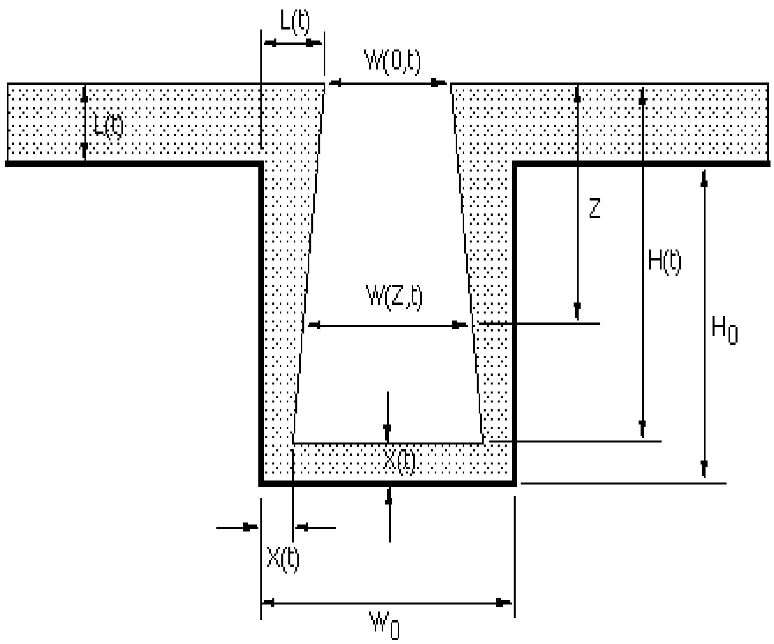
Outline

- LPCVD as a Constrained Optimal Control Problem
  - — Step Coverage Model in Features (long trenches)
  - — A Simplified Model via First Order Perturbations
- Constant vs. Variable Deposition Rates
  - — Optimal Temperature Trajectories with Step Coverage Constraints
  - — Optimal Trajectories for the Reactor-Scale Manipulated Variables
- Results and Discussion

Optimal Control and LPCVD

- An Example: Hydrogen Reduction of Tungsten Hexafluoride
- Industry trends: Smaller features, larger wafers
- Single Wafer Reactors to address uniformity, economical and environmental constraints
- Higher deposition rates required for SWR's to achieve desired throughput
- Step coverage limitations: Constant Rate vs. Variable Rate CVD

Deposition Profiles in Trenches



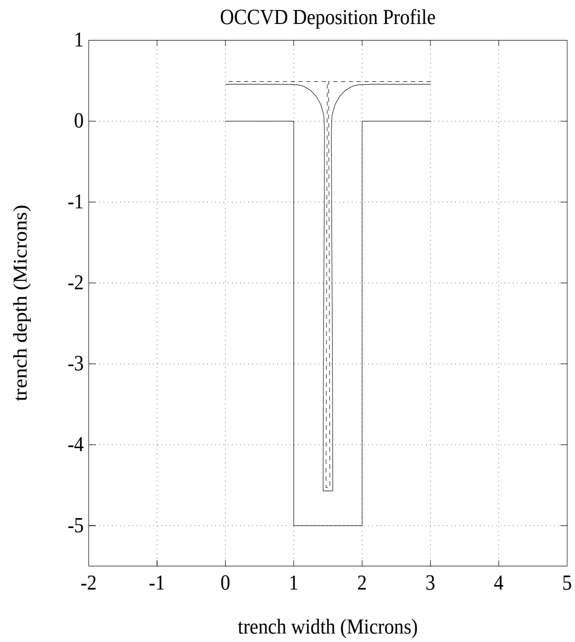


Figure 1: **a.** Idealized cross section of a feature during deposition; **b.** Full model (EVOLVE) vs. Simplified model Comparison

Step Coverage Model

- Heterogeneous reaction and Knudsen diffusion
  - Simpler version of the ballistic transport and reaction model; Integro-differential eqns, better for features

  Assumptions: Deposition rate depends only on limiting reactants, Spatially isothermal feature, Negligible surface diffusion and radial gas concentration gradients ($\Rightarrow$ 1-D process)

- **Reaction:** $3\mathrm{H}_2 + \mathrm{WF}_6 \longrightarrow \mathrm{W}_2 + 6\mathrm{HF}$

$$R(p,T) = k_o \exp\left(-\frac{E_a}{R_g T}\right) \frac{P_{H_2}^{1/2} P_{WF_6}}{1 + k_p P_{WF_6}}, \quad \left(\frac{mol}{cm^2 s}\right)$$

Step Coverage Model (details)

- **Species balance:** (dimensionless)

$$\begin{aligned}\frac{\partial \theta_{WF_6}}{\partial \tau} &= \frac{\mathcal{D}_{WF_6}(0,0)}{\mathcal{D}_H(0,0)} \frac{1}{\mathcal{W}\mathcal{H}^2} \frac{\partial}{\partial \xi}\left(\mathcal{D}\mathcal{W}\frac{\partial \theta_{WF_6}}{\partial \xi}\right) + \frac{P_{H_2}(0,0)}{P_{WF_6}(0,0)} \frac{\phi G}{\mathcal{W}} \\ \frac{\partial \theta_{H_2}}{\partial \tau} &= \frac{1}{\mathcal{W}\mathcal{H}^2} \frac{\partial}{\partial \xi}\left(\mathcal{D}\mathcal{W}\frac{\partial \theta_{H_2}}{\partial \xi}\right) + \frac{3}{\mathcal{W}}\phi G\end{aligned}$$

- **Boundary conditions:**

$$\begin{aligned}\theta_{H_2}(\xi_m,\tau) &= \frac{P_{H_2}(x_m,t)T(0)}{P_{H_2}(0,0)T(t)} \\ \theta_{WF_6}(\xi_m,\tau) &= \frac{P_{WF_6}(x_m,t)T(0)}{P_{WF_6}(0,0)T(t)} \\ \frac{\partial \theta_{H_2}(\xi_b,\tau)}{\partial \xi} &= \frac{3\mathcal{H}(\tau)}{2\alpha_o \mathcal{D}(\xi_b,\tau)}\phi(\tau)G(\xi_b,\tau) \\ \frac{\partial \theta_{WF_6}(\xi_b,\tau)}{\partial \xi} &= \frac{\mathcal{D}_{WF_6}(0,0)}{\mathcal{D}_H(0,0)} \frac{P_{H_2}(0,0)}{P_{WF_6}(0,0)} \frac{\mathcal{H}(\tau)}{2\alpha_o \mathcal{D}(\xi_b,\tau)}\phi(\tau)G(\xi_b,\tau)\end{aligned}$$

- **Initial conditions:**

$$\mathcal{H}(0) = 1 \ ; \quad \theta_H(\xi,0) = 1 \ ; \quad \theta_{WF_6}(\xi,0) = 1 \ ; \quad 0 \le \xi \le 1$$

τ: time; ξ: axial distance; θ: concentration; $\mathcal{W}$: feature width; $\mathcal{H}$: feature depth; $\mathcal{D}$: Knudsen diffusivity; G: rate of reaction, ϕ: step coverage modulus

A Simplified Step Coverage Model

- Quasi-steady-state model, first order perturbation solution

$$\frac{d}{dt}L = R(p(Z,T),T) \;\; ; \;\; \frac{d}{dt}X = \Gamma(t;T)R(p(Z,T),T)$$

Γ: Instantaneous differential step coverage

$$\Gamma(t;T) = \beta(t;T)\frac{1 + k_p P_{WF_6}(x_m,t)}{1 + k_p \beta(t;T) P_{WF_6}(x_m,t)}$$

$$\beta(t;T) = 1 + \frac{4}{C_{WF_6}(0,0)T(0)}\left(\frac{P_{H_2}(0,0)}{P_{WF_6}(0,0)8K_B}\right)^{1/2} T^{1/2}(\alpha+1)\varphi(\alpha)R(p(0,t),T(t)$$

$$\varphi(\alpha) = \frac{18 + 16\alpha(Z,t) + 2\alpha^2(Z,t)}{18 + 7\alpha(Z,t)} \; ; \quad \alpha: \text{ aspect ratio}$$

Constant Rate CVD (CRCVD)

- Minimize processing time (t_f) subject to a step coverage constraint

$$\frac{X(t_f)}{L(t_f)} \geq SC$$

- Assume Constant Partial Pressures at the wafer surface
- Constant temperature (and rate) (CRCVD): Solve for the maximum constant temperature that meets the step coverage constraint (e.g., via line search on either the full or the simplified models).

Optimally Controlled CVD (OCCVD)

- An optimal control (minimum time) problem for the simplified model:

$$\min_{T\in\Omega} t_f$$
$$\text{s.t.}\quad \frac{d}{dt}L = R(p(Z,T),T) \;\; ; \;\; \frac{d}{dt}X = \Gamma(t;T)R(p(Z,T),T)$$
$$X(0) = L(0) = 0 \; ; \;\; \frac{X(t_f)}{L(t_f)} \geq \text{SC} \; ; \;\; L(t_f) = L_*$$

— Constant partial pressures at the wafer surface (optimal trajectories of temperature and partial pressures could be computed in a similar manner)

— Numerical solution via a modified variation of extremals method

OCCVD Computational Procedure

- **Leg 1:** T from the solution of the optimal control problem
- **Leg 2:** Switch to constant T for a fixed time interval (until closure)

Remark: Simplified model deteriorates rapidly near closure

- **Algorithm:** Select time for Leg 2 and repeat until convergence

1. Guess $T(t_f)$ and Integrate 2nd leg backwards to obtain $X(t_f)$
2. Optimal control iteration to find t_f and costates at t_0
3. 1st leg integration to find $T(t_f)$

OCCVD Temperature Trajectory

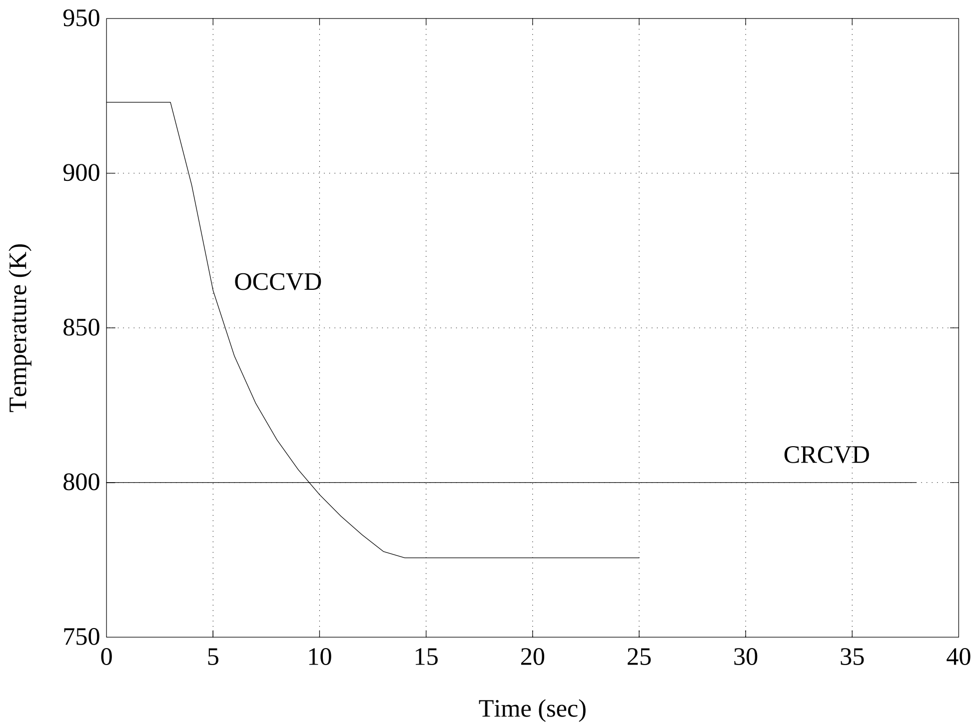


Figure 2: Processing Times and Temperature Trajectories under CRCVD and OCCVD

Simulation Results

- Partial Pressures: $P_{WF_6} = 0.125$ torr, $P_{H_2} = 1.875$ torr. Trench size: $0.7 \times 3\ \mu m$.

  Temperature range constraints: $360 - 650(^oC)$ or $633 - 923(K)$.

- Savings in processing time (SC=0.995, 95 % closure)

  CRCVD: 38 sec. OCCVD: 25 sec. (34% savings)

- Similar results in simulations with the "full" model (EVOLVE; differences within 5 %)

- Different processes or operating conditions produce different time savings

  For example, in thermally activated deposition of SiO_2 from TEOS, CRCVD requires 729 sec. while OCCVD requires only 278 sec.

Reactor Scale Control

- The "desired" processing conditions at the wafer surface (P_{WF_6}, P_{H_2}, T) should be achieved by manipulating external variables (inlet flowrates of H_2, WF_6, total pressure, Temperature/Power)
- With constant inlet flowrates and pressure, temperature variations result in variations of the partial pressures at the wafer surface
- Our Simplified Problem (a small step towards reality):

  Given the desired trajectories for partial pressures and temperature at the wafer surface, generate desired trajectories for total pressure and inlet H_2 flowrate

Reactor Scale Control: Computations

- Constant WF_6 inlet flowrate
- Inner loop controllers (mass flow, temperature) are assumed to be capable to follow the resulting trajectories
- Empirical (but physically motivated) model $(P_0, F_{H_2}, T) \mapsto (P_{WF_6}, P_{H_2})$:

$$
\begin{aligned}
P_{WF_6} &= q_{11} + q_{12}T + q_{13}F_{H_2} + q_{14}\frac{P_0}{1 + F_{H_2}} \\
P_{H_2} &= q_{21} + q_{22}T + q_{23}F_{H_2} + q_{24}\frac{P_0 F_{H_2}}{1 + F_{H_2}}
\end{aligned}
$$

P_0: Total pressure; F_{H_2}: H_2 inlet flowrate

Reactor Scale Control: Computations (cont.)

- The model parameters q_{ij} are updated via Least Squares fit of the model predictions and CFDSWR test-bed simulation results
- The manipulated variable trajectories (P_0, F_{H_2}, T) are generated by recursively solving the above set of nonlinear equations (with the updated coefficients) using Newton's method
- Currently an "open-loop" approach; could be extended to produce a closed-loop design using other measurable quantities (e.g., deposition rates, outlet concentrations) from which the H_2, WF_6 partial pressures at the wafer surface can be inferred

Simulation Results: Controlled vs. Uncontrolled Reactor

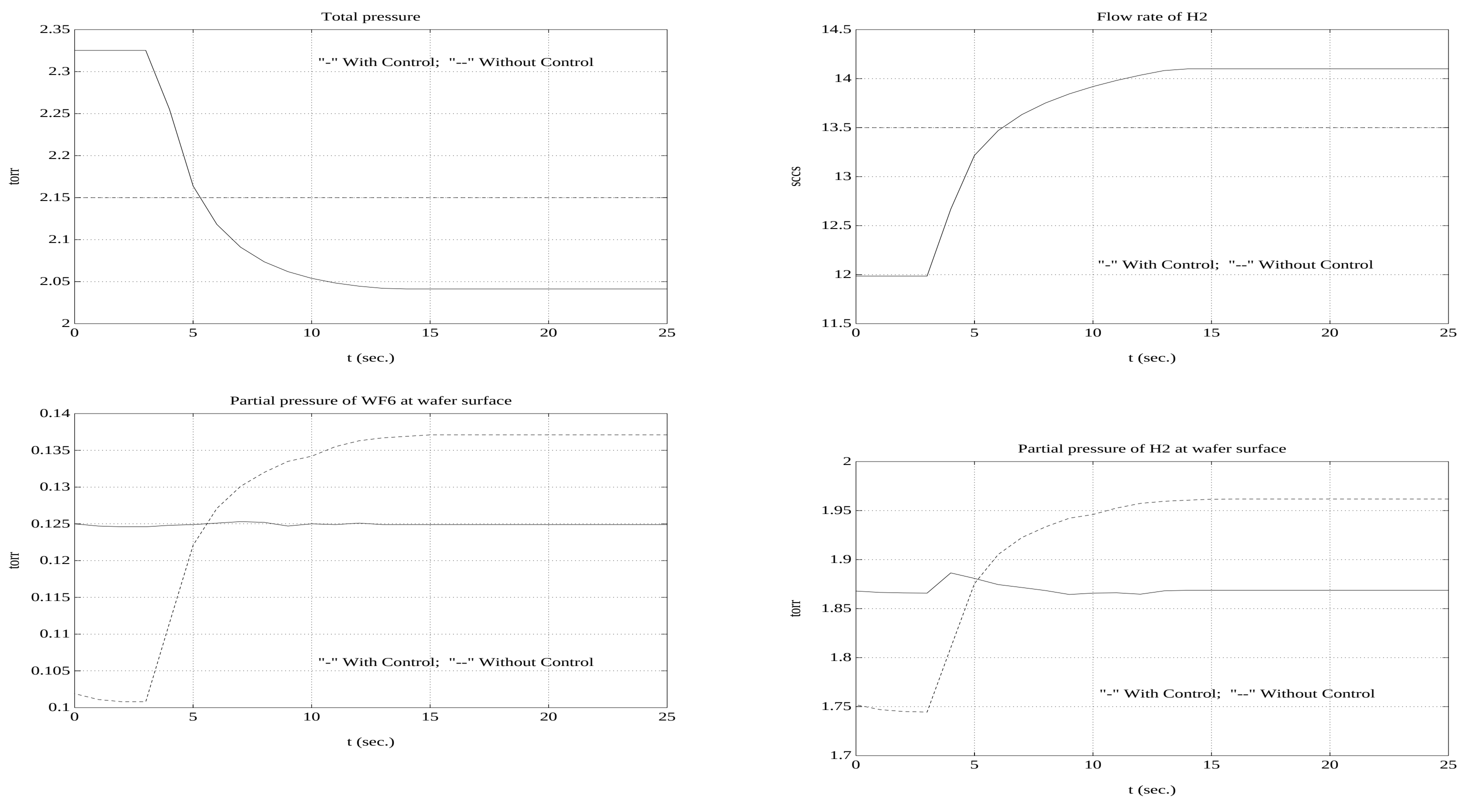


Figure 3: Comparison of constant versus controlled trajectories of Total Pressure and H_2 Inlet Flowrate and the resulting partial pressure trajectories for WF_6 and H_2 at the wafer surface (Control Objective: maintain the desired partial pressures of WF_6 and H_2 at the wafer surface.)

Simulation Results (cont.)

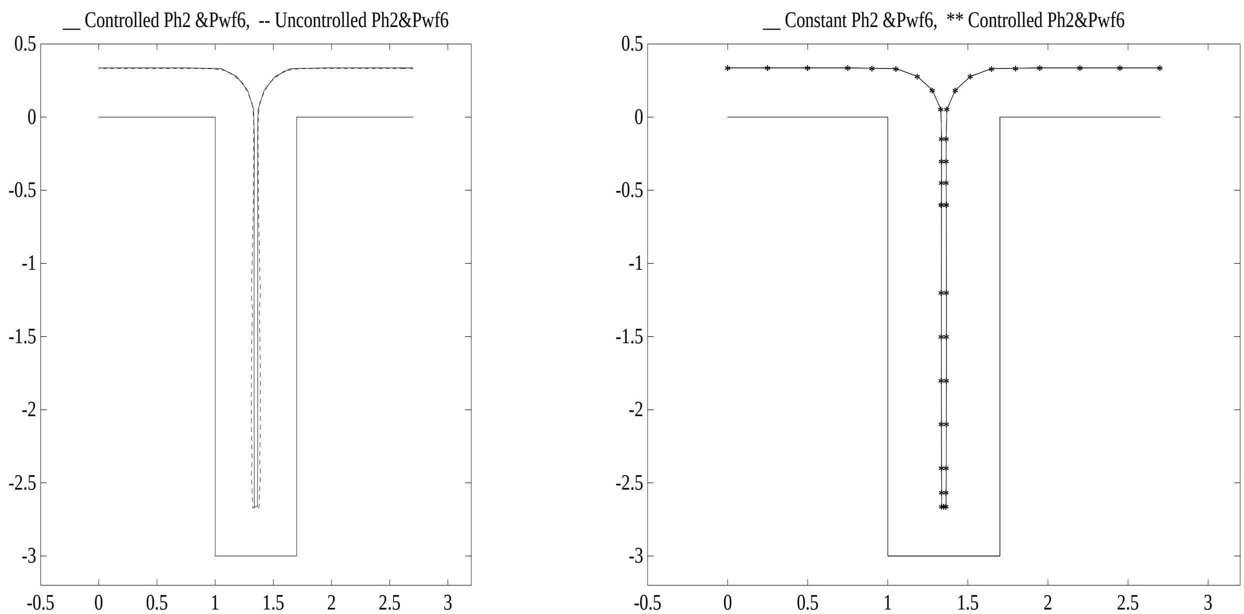


Figure 4: Comparison of resulting deposition profiles (EVOLVE simulation): Constant versus Controlled Reactor variables (Total Pressure and H_2 Inlet Flowrate)

Discussion

- Application of optimal control in CVD can yield significant savings in processing time
- General and systematic approach to compute optimal processing conditions
- Additional constraints on temperature range and rate can be easily incorporated
- Can also address economic efficiency and toxic waste reduction (modification of the cost objective)

Future Considerations

- Experimental validation
- Quality of deposited film (stress, grain size, adhesion, etc.); new models and spec's may be required (process-specific)
- Optimal trajectories for temperature and partial pressures
- Reactor-scale/feature-scale iteration; incorporation of additional reactor scale dynamics and control input constraints (range, rate) in the computation of the optimal trajectories; feasibility of following the desired trajectories (a classical control theory problem)