NONLINEAR MODEL REDUCTION AND CONTROL OF DISTRIBUTED PROCESSES

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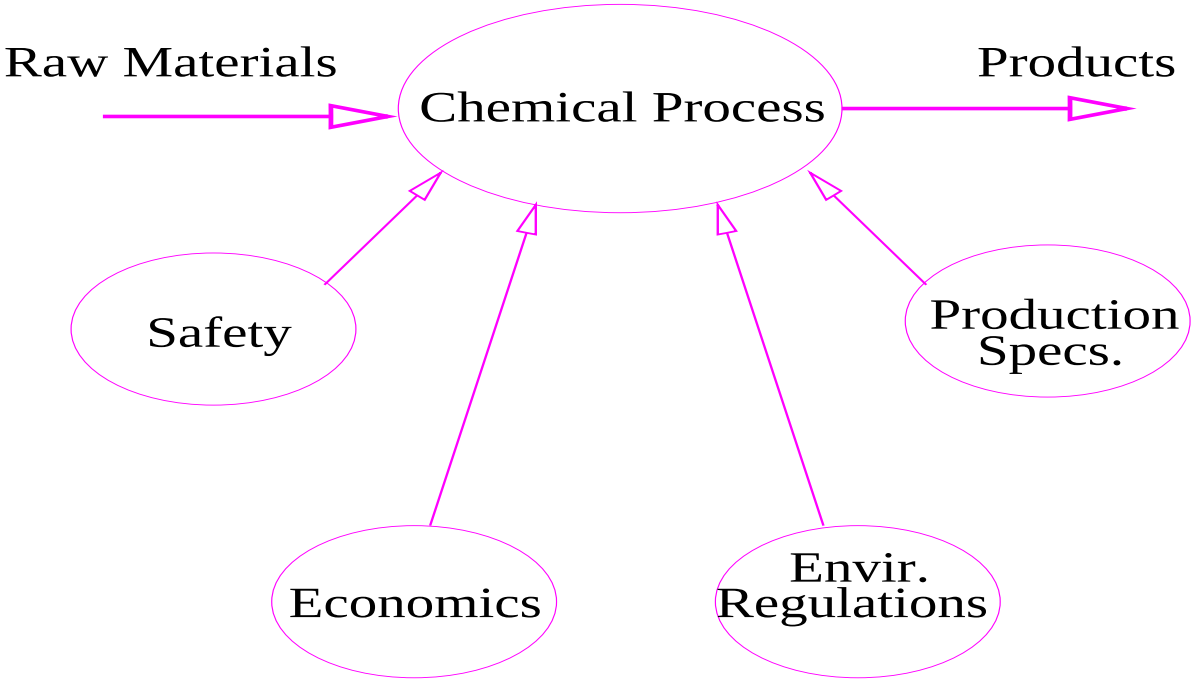
INTRODUCTION

- Incentives for chemical process control.



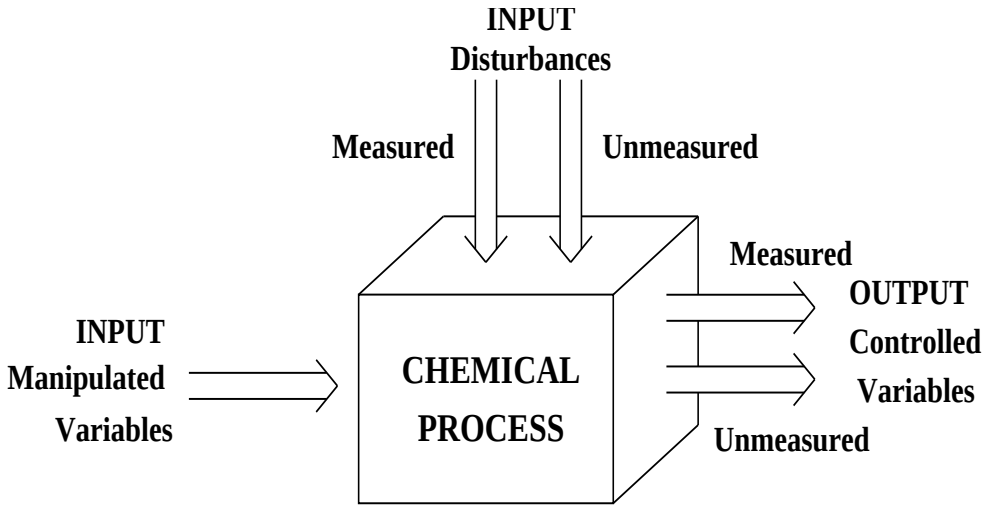
  - ◇ Need for continuous monitoring and external intervention (control).

- Objectives of a process control system.

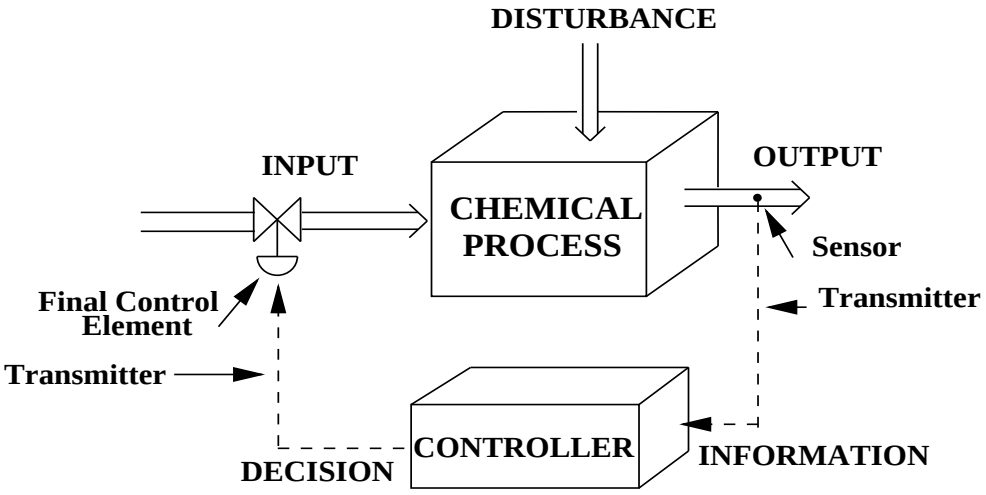
  - ◇ Ensuring stability of the process.
  - ◇ Suppressing the influence of external disturbances.
  - ◇ Optimizing process performance.

BASIC CONCEPTS IN PROCESS CONTROL

- Process variables.

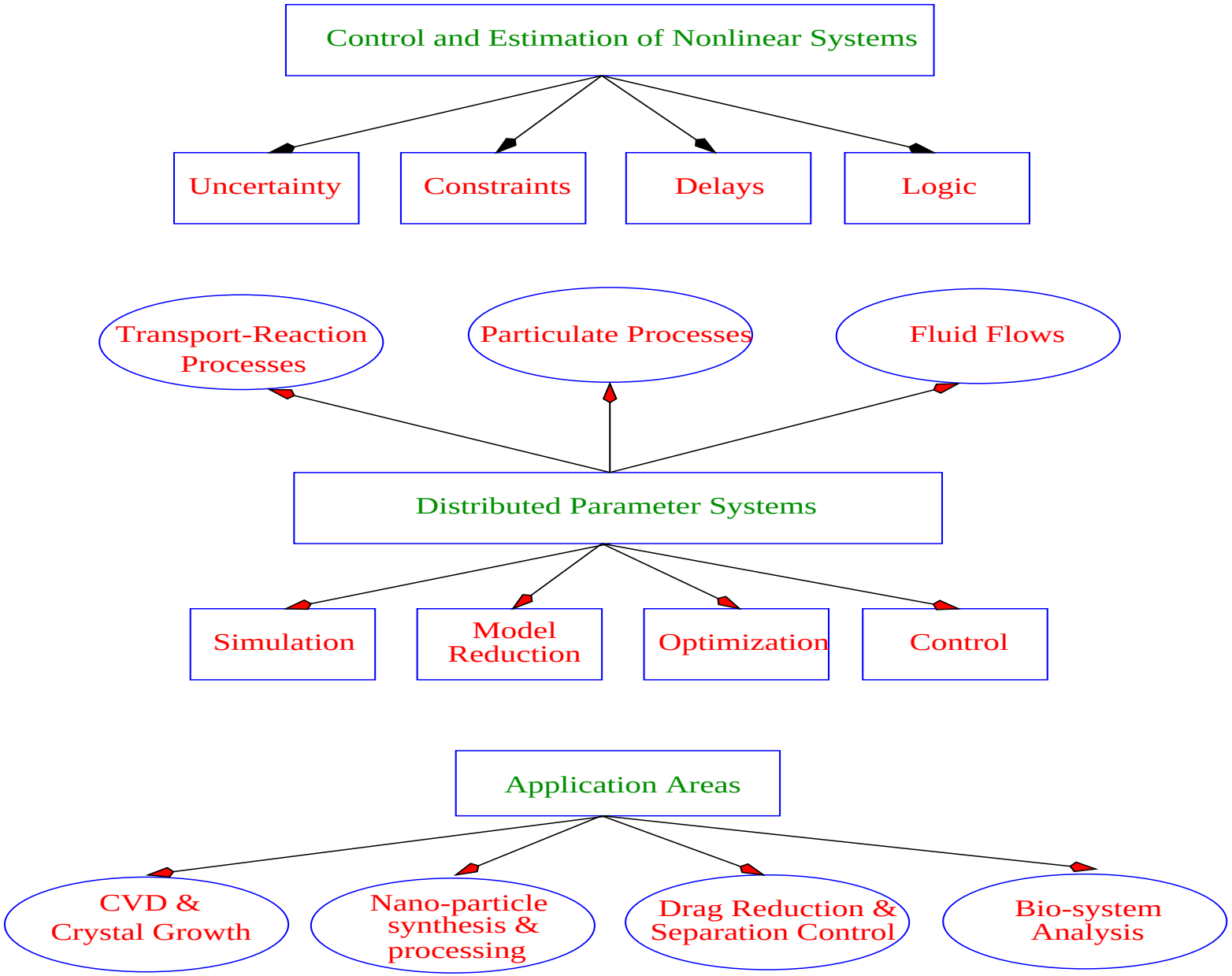


- Feedback control loop.



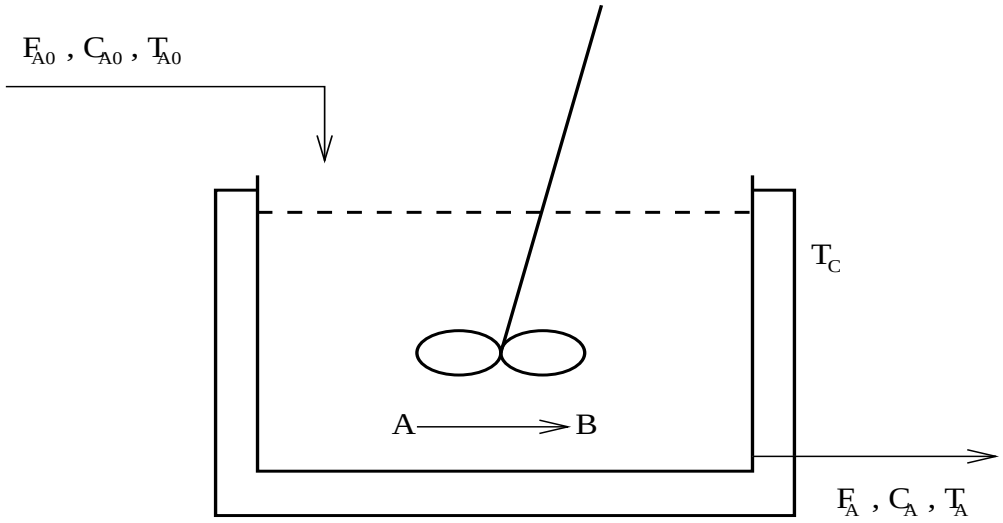
◇ Controller synthesis based on a fundamental process model.

PROCESS CONTROL RESEARCH IN OUR GROUP



LUMPED CHEMICAL PROCESSES

- Example: continuous stirred tank reactor.



- Models: Systems of nonlinear ordinary differential equations.

$$\begin{aligned} \frac{dx}{dt} &= f(x) + g(x)u \\ y &= h(x) \end{aligned}$$

- Approaches for nonlinear controller design.
  - ◇ Geometric control.
  - ◇ Lyapunov-based control.
  - ◇ Model predictive control.

DISTRIBUTED CHEMICAL PROCESSES

- Diffusion-convection-reaction processes.
  - ◇ Control of spatially-distributed profiles.
- Processes with coupled macroscopic and microscopic phenomena.
  - ◇ Control of material microstructure.
- Fluid dynamic systems.
  - ◇ Control for wave suppression, drag reduction and delay of separation.
- Particulate processes.
  - ◇ Control of particle size distribution.

- Typical process models:
  - ◇ Nonlinear parabolic partial differential equations (PDEs).
  - ◇ Coupled PDE and molecular dynamics / Monte-Carlo models.
  - ◇ Navier-Stokes equations.
  - ◇ Nonlinear integro-differential equations.

HISTORICAL PERSPECTIVE

- 1950s and 1960s: lumping.
  - ◇ Distributed nature is neglected.
- 1970s and up to mid 1980s: optimal control (Ray, 1981).
  - ◇ Formulations for linear/nonlinear distributed systems.
  - ◇ Infinite-dimensional controllers / high-order discretizations.
  - ◇ Linearization is typically employed to speed up calculations.
- mid 1980s to mid 1990s: almost no activity.
  - ◇ Control of nonlinear finite-dimensional systems.
- mid 1990s: resurgence of interest.
  - ◇ New actuation / sensing techniques that allow control of distributed objectives become available.
  - ◇ Need to actively control spatial profiles, material microstructure, aerodynamic flows and size distributions becomes clear.

PARABOLIC PDE SYSTEMS

- Systems of parabolic partial differential equations:

$$\frac{\partial \bar{x}}{\partial t} = A\frac{\partial \bar{x}}{\partial z} + D\frac{\partial^2 \bar{x}}{\partial z^2} + f(\bar{x}) + w\bar{u}(z,t)$$

$$\bar{y}_c(z,t) = k\bar{x}, \quad \bar{y}_m(z,t) = \omega\bar{x}$$

- Boundary conditions:

$$C_1\bar{x}(\alpha,t) + B_1\frac{\partial \bar{x}}{\partial z}(\alpha,t) = R_1, \quad C_2\bar{x}(\beta,t) + B_2\frac{\partial \bar{x}}{\partial z}(\beta,t) = R_2$$

$\bar{x}(z,t)$: state variable

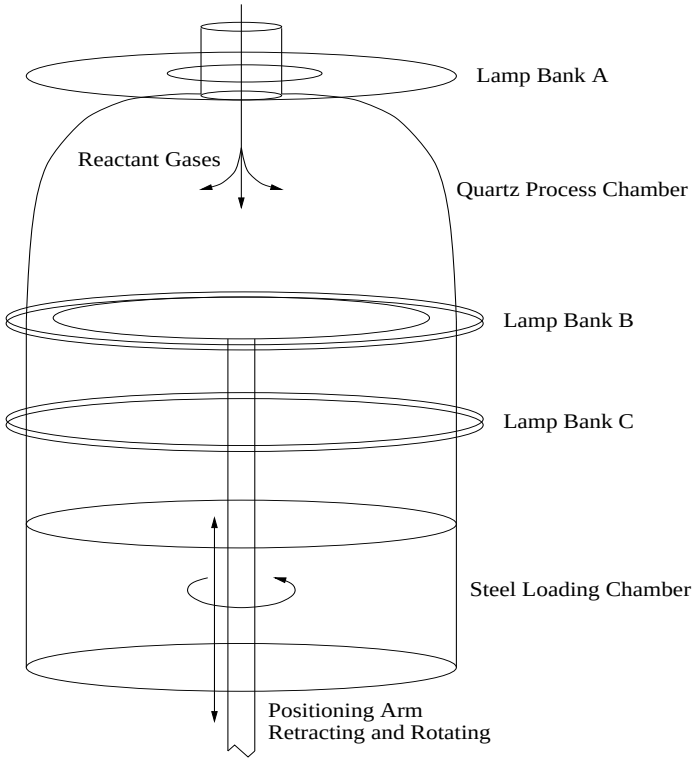
$\bar{u}(z,t)$: manipulated variable

$\bar{y}_m(z,t)$: measured variable

$\bar{y}_c(z,t)$: controlled variable

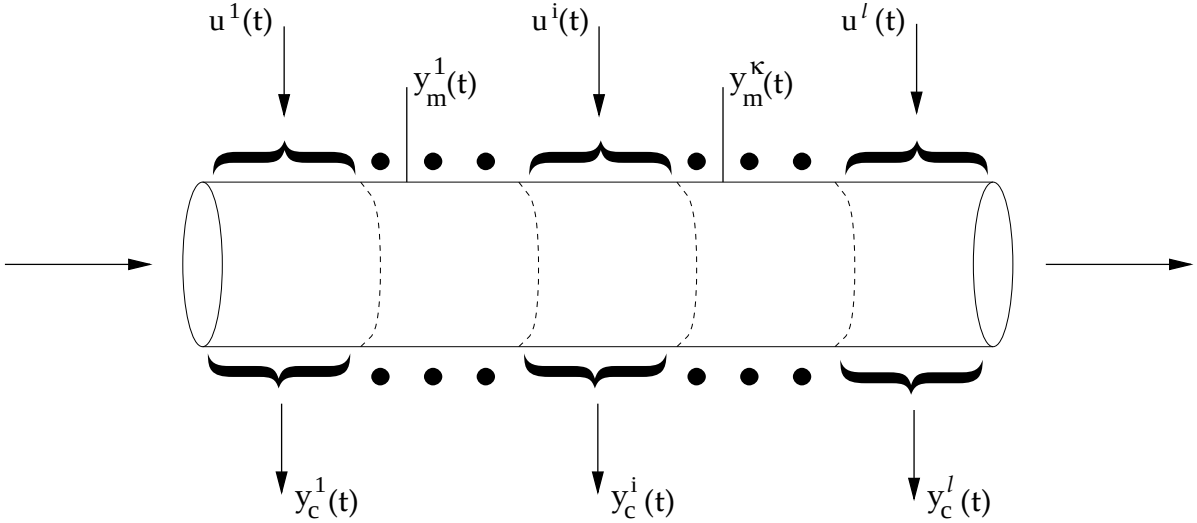
- Boundary control can be included in the above formulation.

RAPID THERMAL CHEMICAL VAPOR DEPOSITION



- Process objective:
  - ◇ Deposit a 0.5 μm polycrystalline silicon thin film on the wafer.
- Operation:
  - ◇ The wafer is heated up to 1200 K with a heating rate of 150 (K/s).
- Control objective:
  - ◇ Manipulate the power of the top lamps to achieve uniform temperature across the wafer.

SPECIFICATION OF THE CONTROL PROBLEM



$u^i(t)$: $i-th$ manipulated input

$b^i(z)$: distribution function of $i-th$ control actuator

$y_c^i(t)$: $i-th$ controlled output

$c^i(z)$: performance specification function

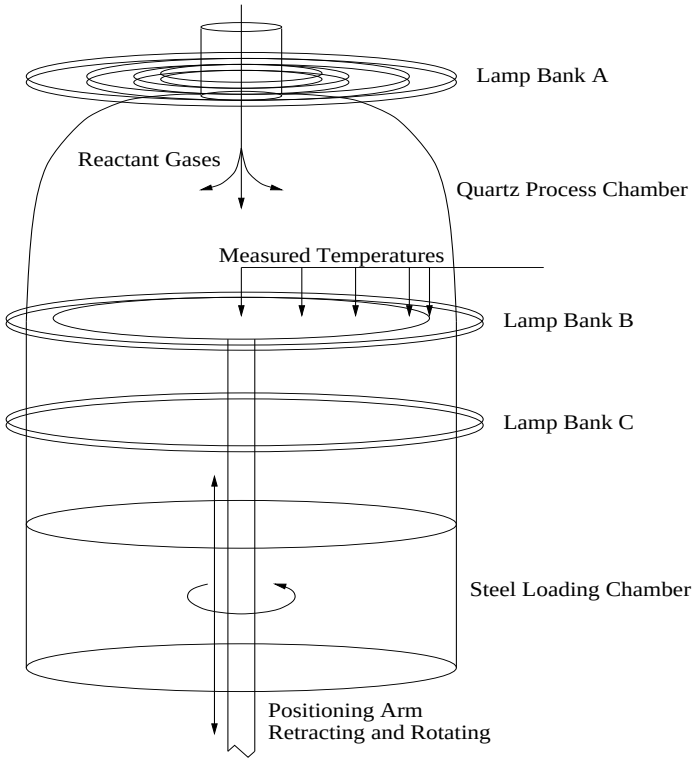
$y_m^\kappa(t)$: $\kappa-th$ measured output

$s^\kappa(z)$: measurement sensor shape function

$$\frac{\partial \bar{x}}{\partial t} = A\frac{\partial \bar{x}}{\partial z} + D\frac{\partial^2 \bar{x}}{\partial z^2} + f(\bar{x}) + w\sum_{i=1}^{l} b^i(z)u^i(t)$$

$$y_c^i(t) = \int_\alpha^\beta c^i(z)k\bar{x}(z,t)dz,\ y_m^\kappa(t) = \int_\alpha^\beta s^\kappa(z)\omega\bar{x}(z,t)dz$$

RAPID THERMAL CHEMICAL VAPOR DEPOSITION



- Control problem specification:
  - ◇ Four concentric independently-controlled lamps are used on the top.
  - ◇ Control of temperature profile across the wafer.
  - ◇ Temperature measurements at five locations across the wafer are available.

PROPERTIES OF PARABOLIC PDEs

- Parabolic PDEs:

$$\frac{\partial \bar{x}}{\partial t} = A\frac{\partial \bar{x}}{\partial z} + D\frac{\partial^2 \bar{x}}{\partial z^2} + f(\bar{x}) + w\sum_{i=1}^{l} b^i(z)u^i(t)$$

- Eigenvalue problem:

$$A\frac{\partial \phi_i}{\partial z} + D\frac{\partial^2 \phi_i}{\partial z^2} = \lambda_i \phi_i$$

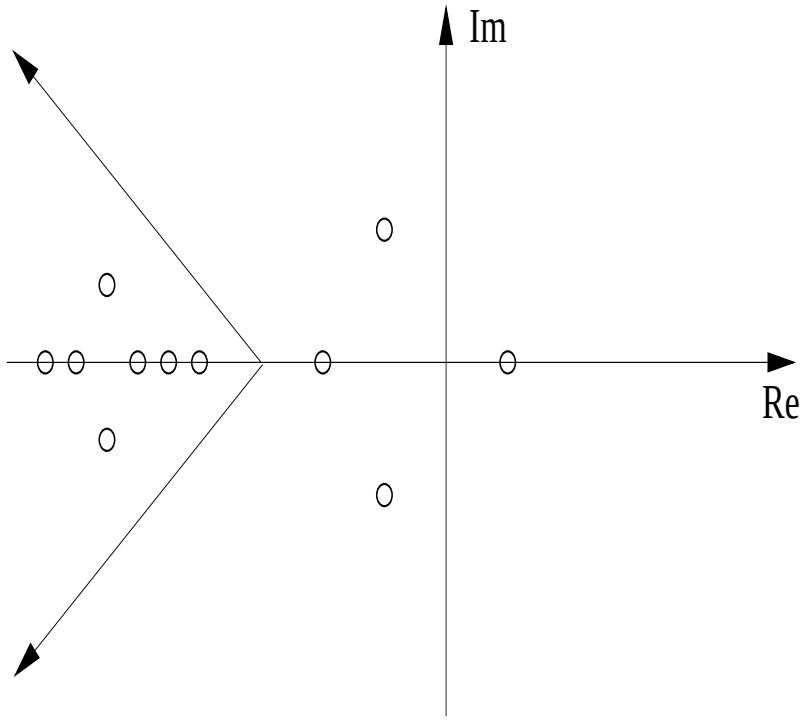
$$C_1\phi_i(\alpha) + B_1\frac{\partial \phi_i}{\partial z}(\alpha) = R_1,$$

$$C_2\phi_i(\beta) + B_2\frac{\partial \phi_i}{\partial z}(\beta) = R_2$$

λ_i: eigenvalue; ϕ_i: eigenfunction.

PROPERTIES OF PARABOLIC PDEs

- Typical structure of eigenspectrum:



- A finite number of dominant modes practically determines the system dynamics.

NONLINEAR CONTROL OF PARABOLIC PDEs

(Christofides, Birkhäuser, 2001)

- Derivation of low-dimensional ODE models.
  - ◇ Singular perturbation formulation of Galerkin's method.
  - ◇ Inertial manifolds and approximate inertial manifolds.
- Feedback controller synthesis.
  - ◇ Nonlinear control methods for ODE systems.
- Characterization of closed-loop stability and transient performance.
  - ◇ Singular perturbations and Lyapunov techniques.

GALERKIN'S METHOD

- $\mathcal{H}_s = span\{\phi_1, \phi_2, \ldots, \phi_m\}$, $\mathcal{H}_f = span\{\phi_{m+1}, \phi_{m+2}, \ldots, \}$.

$$x_s(t) = P_s x(t), \quad x_f(t) = P_f x(t)$$

P_s, P_f: orthogonal projection operators.

x_s: state vector corresponding to slow eigenmodes.

x_f: state vector corresponding to fast eigenmodes.

- Set of infinite ODEs.

$$\begin{aligned} \frac{dx_s}{dt} &= A_s x_s + b_s u + f_s(x_s, x_f) \\ \frac{\partial x_f}{\partial t} &= A_f x_f + b_f u + f_f(x_s, x_f) \end{aligned}$$

GALERKIN'S METHOD

Singular Perturbation formulation

- $\epsilon = \dfrac{|Re\lambda_1|}{|Re\lambda_{m+1}|} < 1.$

$$\begin{aligned} \frac{dx_s}{dt} &= A_s x_s + b_s u + f_s(x_s, x_f) \\ \epsilon \frac{\partial x_f}{\partial t} &= A_{f\epsilon} x_f + \epsilon b_f u + \epsilon f_f(x_s, x_f) \end{aligned}$$

- Setting $\epsilon = 0$:

$$\begin{aligned} \frac{d\bar{x}_s}{dt} &= A_s \bar{x}_s + b_s u + f_s(\bar{x}_s, 0) \\ \bar{x}_f &= 0 \end{aligned}$$

- Closeness of solutions ($u(t) \equiv 0$, ϵ sufficiently small):

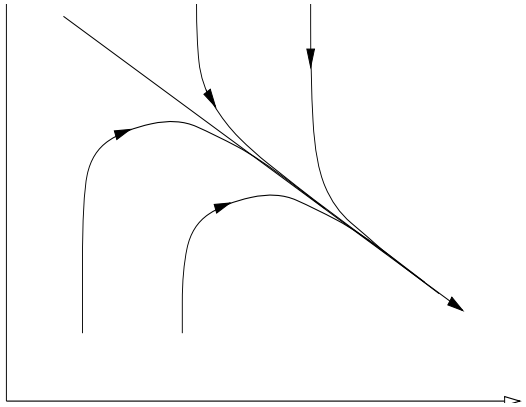
  - $||x - \bar{x}_s||_2 = O(\epsilon)$, $\forall\ t \geq 0$.

High-dimensionality of the ODE system for desired accuracy?

INERTIAL MANIFOLD

- Inertial manifold: a finite-dimensional invariant manifold M:

$$x_f = \Sigma(x_s, u, \epsilon)$$



- On M the solutions are exactly described by the ODE slow system:

$$\frac{dx_s}{dt} = A_s x_s + b_s u + f_s(x_s, \Sigma(x_s, u, \epsilon))$$

- $\Sigma(x_s, u, \epsilon)$ is the solution of:

$$\epsilon \frac{\partial \Sigma}{\partial x_s}[A_s x_s + b_s u + f_s(x_s, x_f)] + \epsilon \frac{\partial \Sigma}{\partial u}\dot{u} = A_{f\epsilon} x_f + \epsilon b_f u + \epsilon f_f(x_s, x_f)$$

APPROXIMATE INERTIAL MANIFOLDS

- Procedure for the construction of approximations of $\Sigma(x_s, u, \epsilon)$.

  - ◇ Series expansion in ϵ.

$$
\begin{aligned}
u(x_s, \epsilon) &= u_0(x_s, \epsilon) + \epsilon u_1(x_s, \epsilon) + \cdots + \epsilon^k u_k(x_s, \epsilon) + O(\epsilon^{k+1}) \\
\Sigma(x_s, u, \epsilon) &= \Sigma^0(x_s, u) + \epsilon \Sigma^1(x_s, u) + \cdots + \epsilon^k \Sigma^k(x_s, u) + O(\epsilon^{k+1})
\end{aligned}
$$

  - ◇ Substitution into the manifold equation.

- Results:

  $O(\epsilon)$ approximation: $\Sigma^0(x_s, u) = 0$.

  $O(\epsilon^2)$ approximation: $\Sigma^1(x_s, u) = (A_f)^{-1}[-b_f u_0 - f_f(x_s, 0)]$.

  ...

APPROXIMATE INERTIAL FORM

- Approximate inertial form.

$$\begin{aligned}
\frac{d\bar{x}_s}{dt} &= A_s\bar{x}_s + b_s u \\
&\quad + f_s(\bar{x}_s, \Sigma^0(\bar{x}_s, u) + \epsilon\Sigma^1(\bar{x}_s, u) + \cdots + \epsilon^k\Sigma^k(\bar{x}_s, u)) \\
y_{cs} &= \mathcal{C}(\bar{x}_s + \Sigma^0(\bar{x}_s, u) + \epsilon\Sigma^1(\bar{x}_s, u) + \cdots + \epsilon^k\Sigma^k(\bar{x}_s, u))
\end{aligned}$$

- Closeness of solutions ($u(t) \equiv 0$, ϵ sufficiently small):

$$||x(t) - \bar{x}_s(t)||_2 = O(\epsilon^{k+1}),\ \forall t \geq t_b,$$

t_b: time required for $x_f(t)$ to approach $\Sigma(x_s, u, \epsilon)$.

NONLINEAR OUTPUT FEEDBACK CONTROL

- Controller synthesis: combination of state feedback with state observers.
  - ◇ State feedback controller synthesis.

$$u = u_0 + \epsilon u_1 + \cdots + \epsilon^k u_k$$

    - ▷ Synthesize u_0 on the basis of $O(\epsilon)$ slow system.
    - ▷ Synthesize u_1 on the basis of $O(\epsilon^2)$ slow system.
    - ▷ ...
  - ◇ State observer:

$$\frac{d\eta}{dt} = A_s\eta + b_s u + f_s(\eta, \Sigma^0(\eta,u) + \epsilon\Sigma^1(\eta,u) + \cdots + \epsilon^k\Sigma^k(\eta,u))$$
$$+L(y_m - \mathcal{S}(\eta + \Sigma^0(\eta,u) + \epsilon\Sigma^1(\eta,u) + \cdots + \epsilon^k\Sigma^k(\eta,u))$$

- Performance characterization:

$$y_c^i(t) = y_{cs}^i(t) + O(\epsilon^{k+1}) \ , \ i = 1, \ldots, l \ , \ t \geq t_b$$

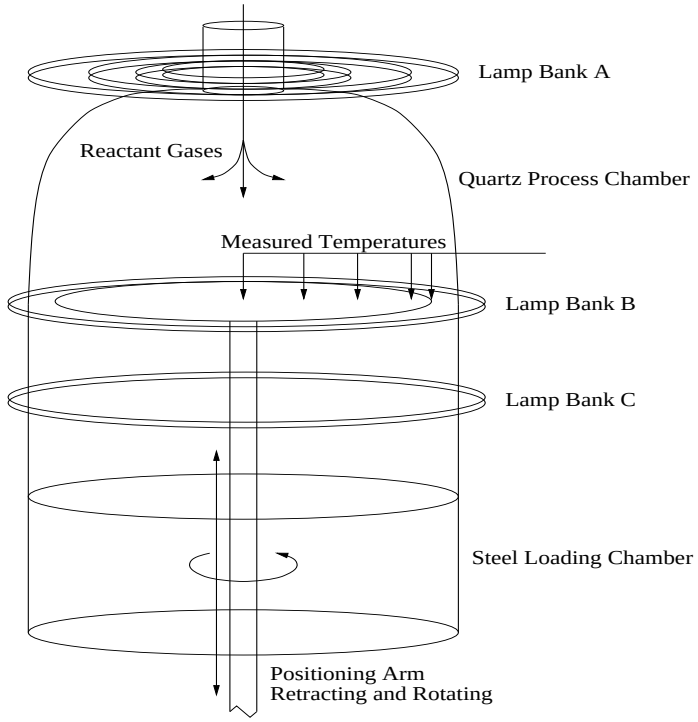
CONTROL OF PARABOLIC PDEs: SUMMARY OF RESULTS

- Robust control of PDEs with uncertainty (Christofides, CES, 1998; Christofides and Baker S & CL, 1999).
- Nonlinear control of PDEs with time-delays (Antoniades and Christofides, IJC, 2000).
- Bounded control of PDEs with actuator saturation (El-Farra, Armaou and Christofides, Automatica, 2003).
- Nonlinear control of PDEs with nonlinear spatial differential operators (Baker and Christofides, I & EC Research, 1999; IJC, 2000).
- Nonlinear and robust control of PDEs with time-dependent spatial domains (Armaou and Christofides, JMAA, 1999; Automatica, 2000; IJAMCS 2001).
- Integration of optimal actuator/sensor placement and nonlinear control (Antoniades and Christofides, C & CE, 2000; CES 2001; C & CE, 2002; IEEE CST, 2003).

APPLICATIONS TO TRANSPORT-REACTION PROCESSES

- Diffusion-reaction processes with various kinetic mechanisms, time-dependent spatial domains and spatially-varying coefficients (Christofides, Birkhäuser, 2001).
  - ◇ Stabilization of spatially-distributed profiles.
- Tubular reactors with/without recycle loops (Antoniades and Christofides, NA, 2001).
  - ◇ Control of reactor temperature profiles.
- Chemical vapor deposition processes (Armaou and Christofides, CES, 1999; Baker and Christofides, IJC, 2000).
  - ◇ Control of wafer temperature profile and deposition rate.
- Czochralski crystallization of high-purity crystals (Armaou and Christofides, AIChE J., 2001).
  - ◇ Crystal temperature and thermal gradient control.

RAPID THERMAL CHEMICAL VAPOR DEPOSITION



- Manipulate the power of the top lamps to achieve uniform temperature across the wafer.
- Four concentric independently-controlled lamps are used on the top.
- Temperature measurements at five locations across the wafer are assumed to be available.
- Low pressure; radiation is the dominant heat transfer mechanism.

RAPID THERMAL CHEMICAL VAPOR DEPOSITION

(e.g., Breedijk *et al.*, ACC, 1993, Theodoropoulou *et al.*, IEEE TSM, 1997)

- Wafer energy balance:

$$\rho_w T_{amb} \frac{\partial}{\partial t}\left(C_{p_w}(T)T\right) = \frac{T_{amb}}{R_w^2}\frac{1}{r}\frac{\partial}{\partial r}\left(\kappa(T) r \frac{\partial T}{\partial r}\right) - \frac{q_{rad}(T,r)}{\delta z}$$

- Boundary conditions:

$$\left.\frac{\partial T}{\partial r}\right|_{r=0} = 0, \quad \left.(\kappa(T)\frac{\partial T}{\partial r})\right|_{r=1} = -\sigma\epsilon_w T_{amb}^4 (T^4 - T_c^4) + q_{edge} u_b$$

- Energy balance on the chamber:

$$T_{amb} M_c \frac{dT_c}{dt} = \epsilon_c Q_{lamps} u - A_{hem}\, q_{hem} - A_{cyl}\, q_{cyl} - Q_{convect}$$
$$-\sigma\epsilon_c A_c T_{amb}^4 (T_c^4 - 1)$$

RAPID THERMAL CHEMICAL VAPOR DEPOSITION

(e.g., Breedijk *et al.*, ACC, 1993, Theodoropoulou *et al.*, IEEE TSM, 1997)

- Mass balances on the chamber:

$$\frac{dX_{SiH_4}}{dt} = -\alpha \int_{A_w} R_s \, dA_w + \frac{1}{\tau}(X^{in}_{SiH_4} - X_{SiH_4})$$

$$\frac{dX_{H_2}}{dt} = 2\alpha \int_{A_w} R_s \, dA_w - \frac{1}{\tau} X_{H_2}$$

- Deposition rate:

$$\frac{dS}{dt} = \frac{MW_{Si}}{\rho_{Si}} \frac{k_0 \, exp\left(\frac{-\gamma}{R \, T \, T_{amb}}\right) X_{SiH_4} P_{tot}}{1 + bX_{SiH_4} P_{tot} + \frac{\sqrt{X_{H_2} P_{tot}}}{c}}$$

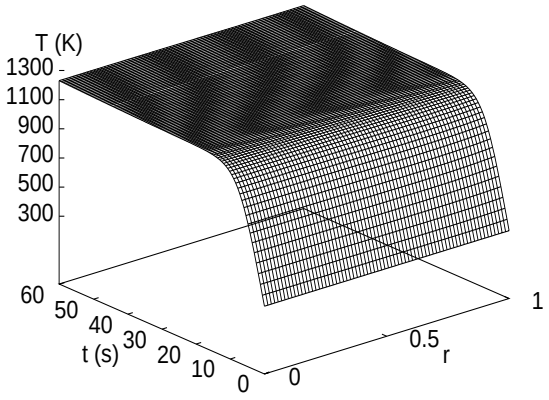
RAPID THERMAL CHEMICAL VAPOR DEPOSITION
Methodology for nonlinear controller design

- Finite-difference method is used to develop a detailed simulation of the process model.
- Data of the detailed process simulation are used to compute the four dominant empirical eigenfunctions via Karhunen-Loeve decomposition.
- Orthogonal collocation formulation of Galerkin's method with 5 collocation points.
- Derivation of a fifth-order ODE model.
- Nonlinear output feedback controller design.

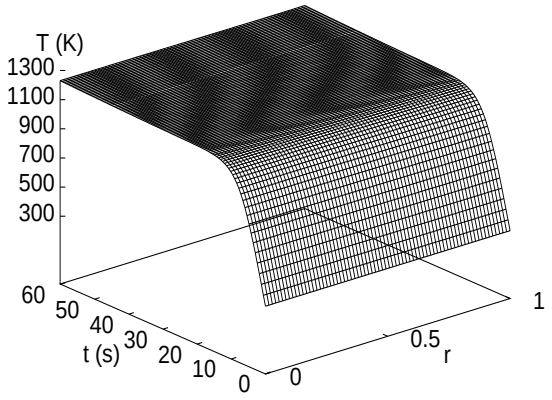
RAPID THERMAL CHEMICAL VAPOR DEPOSITION

Open-loop simulation results

Spatiotemporal wafer temperature profile - a) full model, b) reduced model.

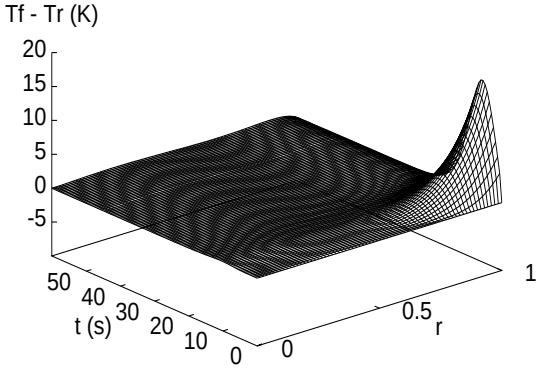


a)



b)

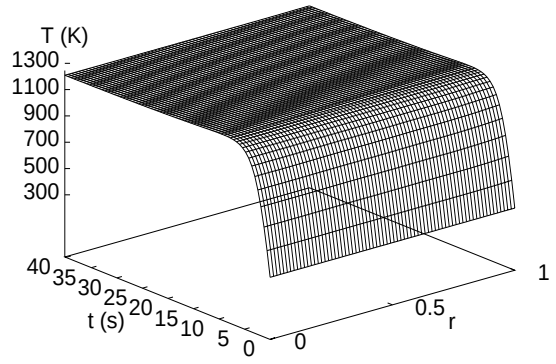
Difference between full and reduced models.



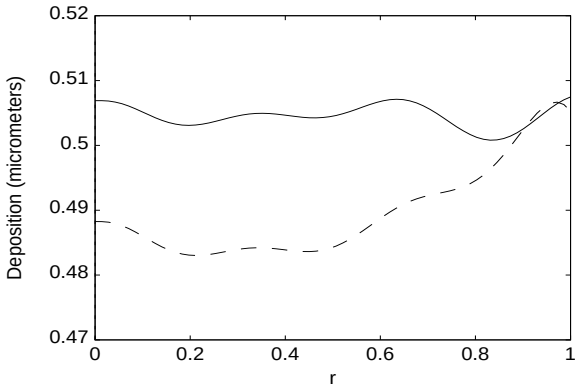
RAPID THERMAL CHEMICAL VAPOR DEPOSITION

Closed-loop simulation results

Spatiotemporal wafer temperature profile under nonlinear control.



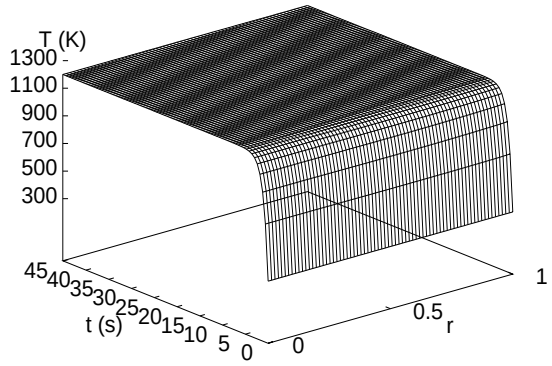
Final film thickness ($t = 40\ sec$) - under nonlinear control (solid line) and PI control (dashed line).



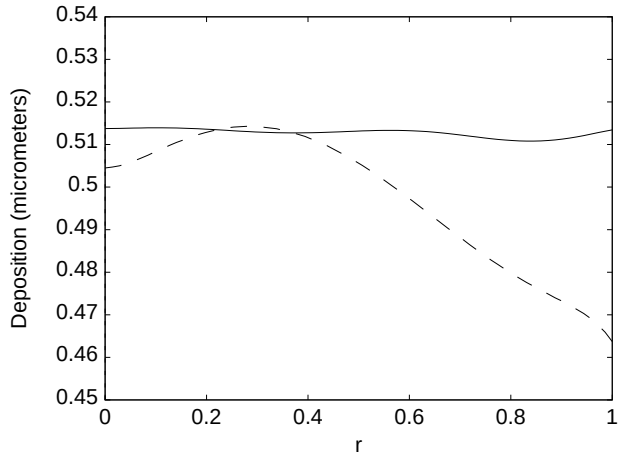
RAPID THERMAL CHEMICAL VAPOR DEPOSITION

Closed-loop simulation results

Spatiotemporal wafer temperature profile under nonlinear control in the presence of uncertainty.

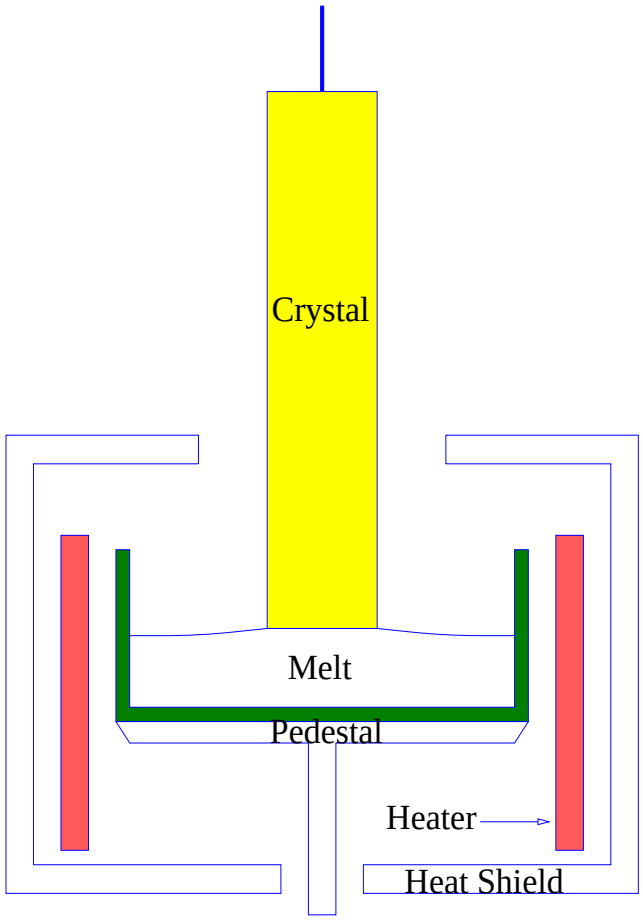


Final film thickness in the presence of uncertainty under nonlinear control (solid line) and PI control (dashed line).



CONTROL OF CZOCHRALSKI CRYSTAL GROWTH

(Armaou and Christofides, AIChE J., 2001)



- Process objective: Growth of a 0.7m silicon crystal.
- Control objective: Smooth axial temperature drop inside the crystal.

CZOCHRALSKI CRYSTAL GROWTH

Mathematical model

- Energy balance on the crystal:

$$\frac{\partial T_c}{\partial t} + u_p \frac{\partial T_c}{\partial z} = \frac{k}{\rho c_p}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T_c}{\partial r}\right) + \frac{\partial^2 T_c}{\partial z^2}\right]$$

- Boundary conditions:

$$T_c(r,0,t) = T_{mp}, \quad 0 \le r \le R$$

$$\left.\frac{\partial T_c}{\partial r}\right|_0 = 0, \quad 0 \le z \le l(t)$$

$$\begin{aligned}\left.\frac{k}{\sigma}\frac{\partial T_c}{\partial r}\right|_R =& \epsilon_{w_{cr}}\epsilon_{w_m} F_{cr\to m}(R,z)[T_m^4 - T_c^4(R,z,t)] \\ &+\epsilon_{w_{cr}}\epsilon_{w_{ch}} F_{cr\to ch}(R,z)[T_{ch}^4 - T_c^4(R,z,t)] \\ &+\epsilon_{w_{cr}}\epsilon_{w_{amb}} F_{cr\to amb}(R,z)[T_{amb}^4 - T_c^4(R,z,t)], \quad 0 \le z \le l(t)\end{aligned}$$

CZOCHRALSKI CRYSTAL GROWTH

Mathematical model

- Boundary conditions:

$$\begin{aligned}\frac{k}{\sigma}\frac{\partial T_c}{\partial z}\bigg|_{l(t)} =& \epsilon_{w_{cr}}\epsilon_{w_m}F_{cr\to m}(r,l(t))[T_m^4 - T_c^4(r,l(t),t)] \\ &+\epsilon_{w_{cr}}\epsilon_{w_{ch}}F_{cr\to ch}(r,l(t))[T_{ch}^4 - T_c^4(r,l(t),t)] \\ &+\epsilon_{w_{cr}}\epsilon_{w_{amb}}F_{cr\to amb}(r,l(t))[T_{amb}^4 - T_c^4(r,l(t),t)], \quad 0 \le r \le R\end{aligned}$$

- Moving boundary:

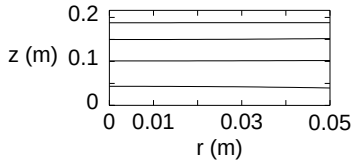
$$l(t) = l(0) + V_p(t)t, \quad V_p(t) = \begin{cases} V_p, & l(t) < l_{max} \\ 0, & l(t) = l_{max} \end{cases},$$

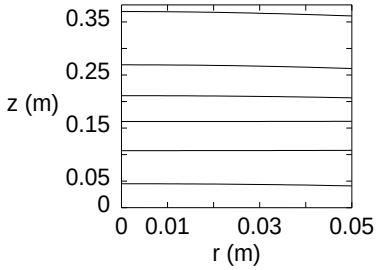
$$l(0) = 0.05\ m, \quad l_{max} = 0.7\ m$$

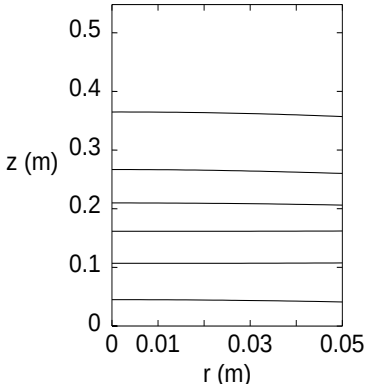
CZOCHRALSKI CRYSTAL GROWTH

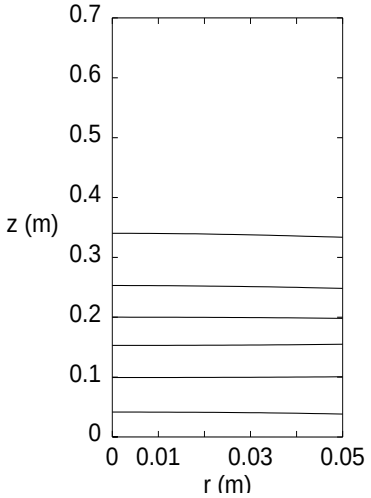
Simulation of open-loop system

Time evolution of crystal temperature profile.



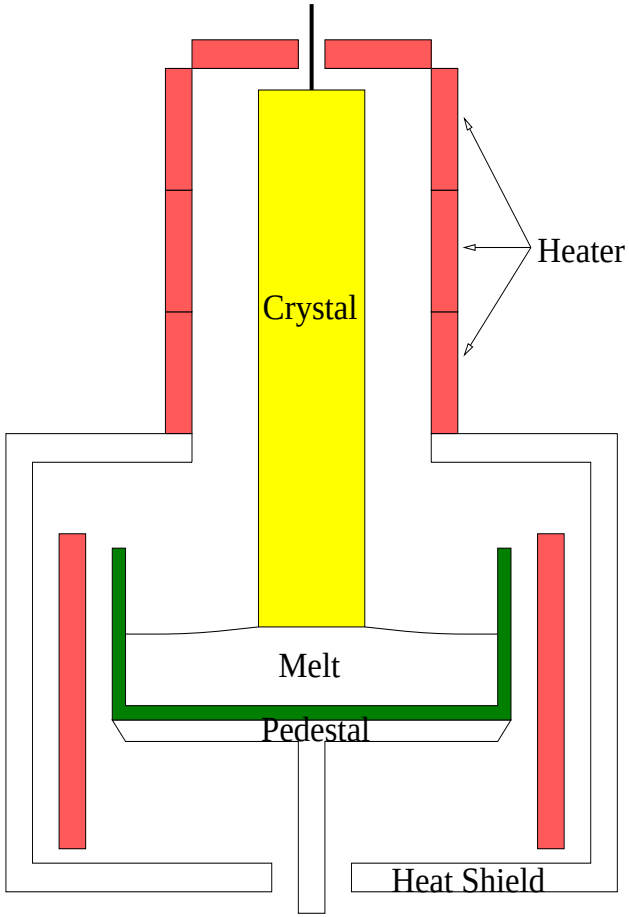






CZOCHRALSKI CRYSTAL GROWTH

Control problem specification

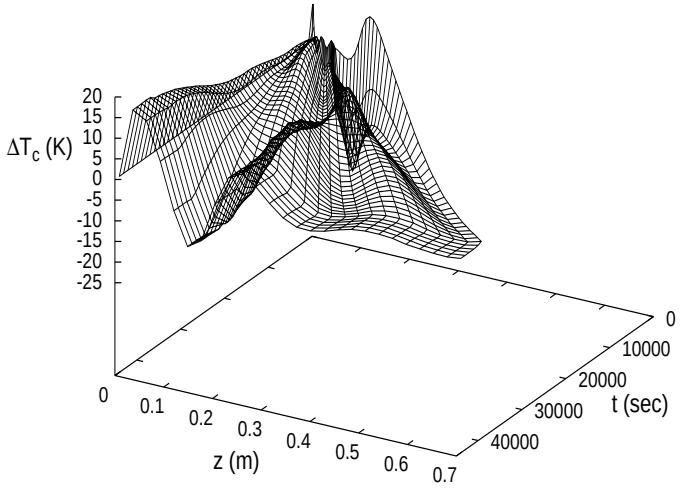


- Heater temperature is used as the manipulated input.
- Control objective: smooth temperature drop along the length of the crystal.
- Three point measurements of the crystal temperature are available.

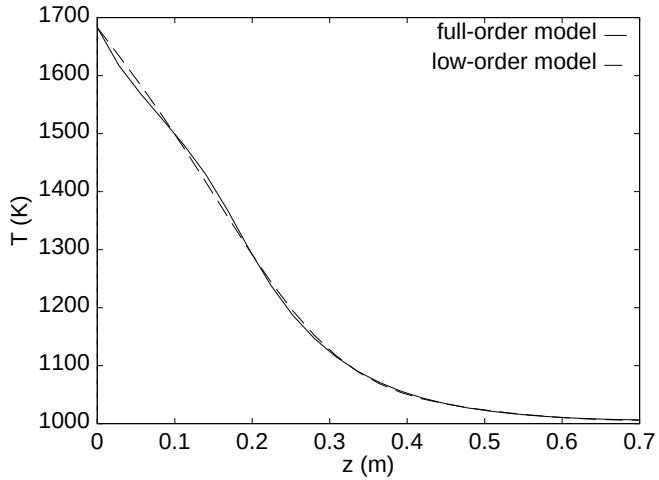
CZOCHRALSKI CRYSTAL GROWTH

Accuracy of Galerkin/AIM: 4/4 approximation

Time evolution of maximum temperature difference.



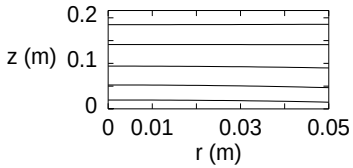
Crystal temperature profile at $t = 45000\ s$.

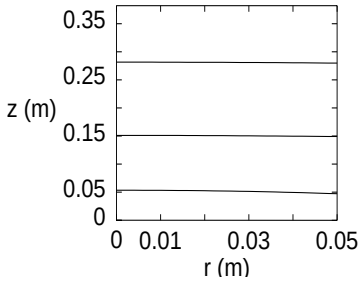


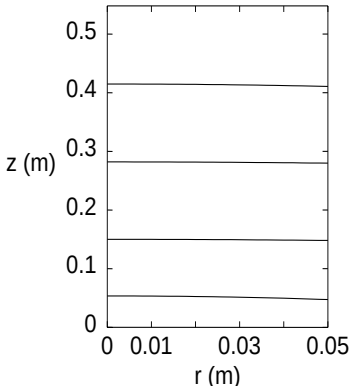
CZOCHRALSKI CRYSTAL GROWTH

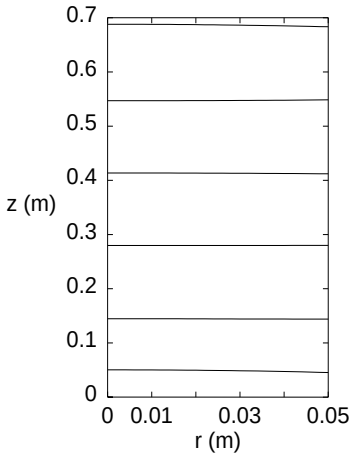
Galerkin/AIM model-based controller: 4/4

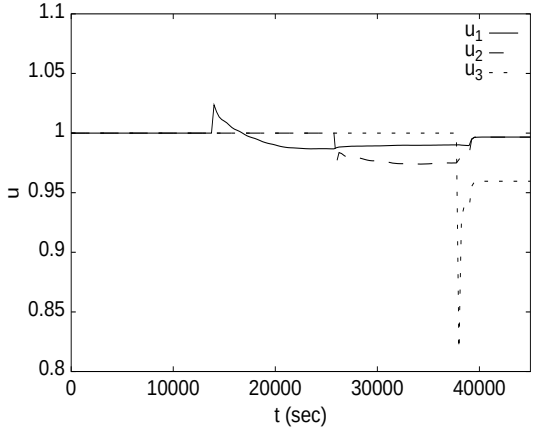
Time evolution of crystal temperature profile - nominal case.









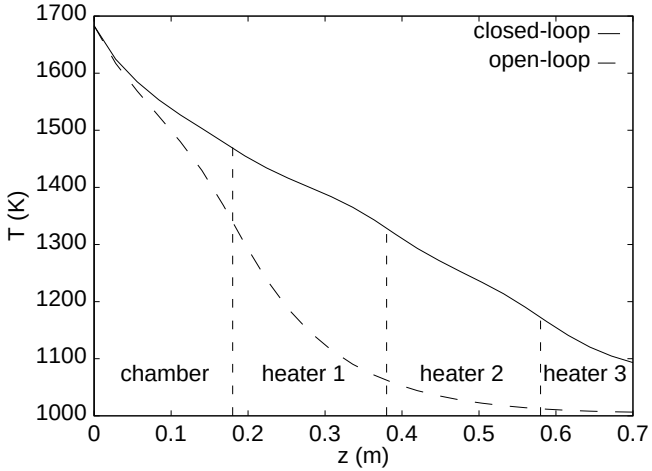


Manipulated inputs: $(u_i(t) = \dfrac{T_i(t)}{T_{sp_i}})$.

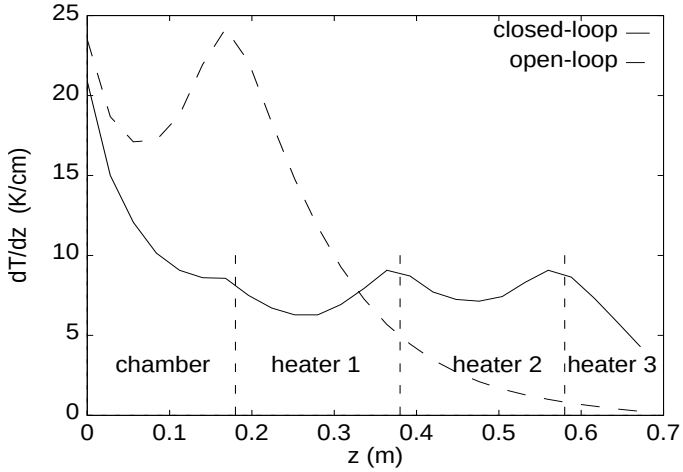
CZOCHRALSKI CRYSTAL GROWTH

Galerkin/AIM model-based controller: 4/4

Crystal temperature profile at $t = 45000\ s$.



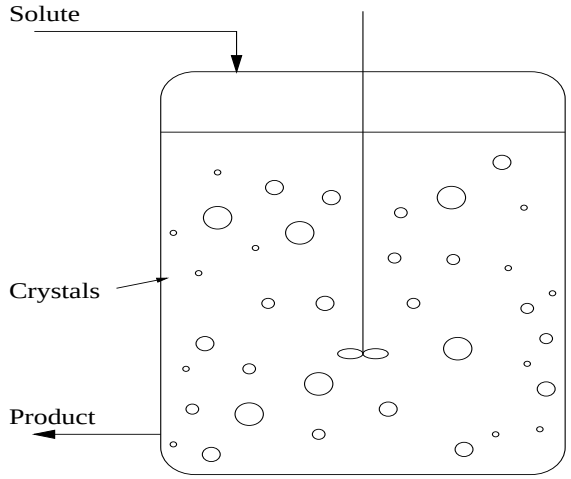
Axial temperature gradient at $t = 45000\ s$.



CONTROL OF PARTICULATE PROCESSES

(Christofides, Kluwer Academic, 2002)

- Example: continuous crystallization.



- Population balance equation:

$$\frac{\partial n}{\partial t} = -\frac{\partial(k_1(c-c_s)n)}{\partial r} - \frac{n}{\tau} + \delta(r-0)\epsilon k_2 exp(-\frac{k_3}{\left(\frac{c}{c_s}-1\right)^2})$$

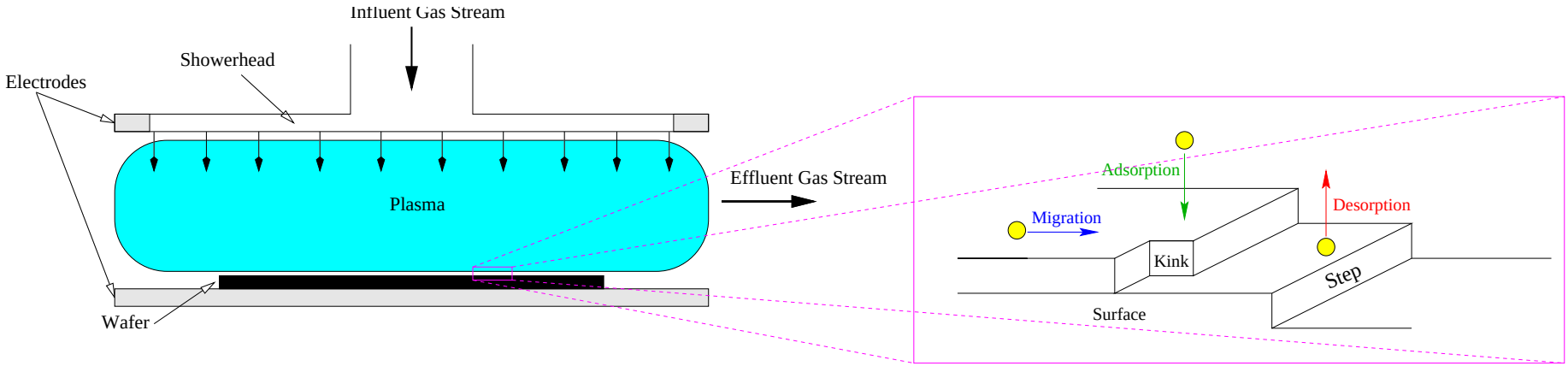
- Mass balance equation:

$$\frac{dc}{dt} = \frac{(c_0-\rho)}{\epsilon\tau} + \frac{(\rho-c)}{\tau} + \frac{(\rho-c)}{\epsilon}\frac{d\epsilon}{dt}, \quad \epsilon = 1 - \int_0^\infty n(r,t)\frac{4}{3}\pi r^3 dr$$

- Control objective: Produce crystals with a desired size distribution.

CONTROL OF THIN FILM MICROSTRUCTURE

(Lou and Christofides, CES, 2003; AIChE J. 2003)



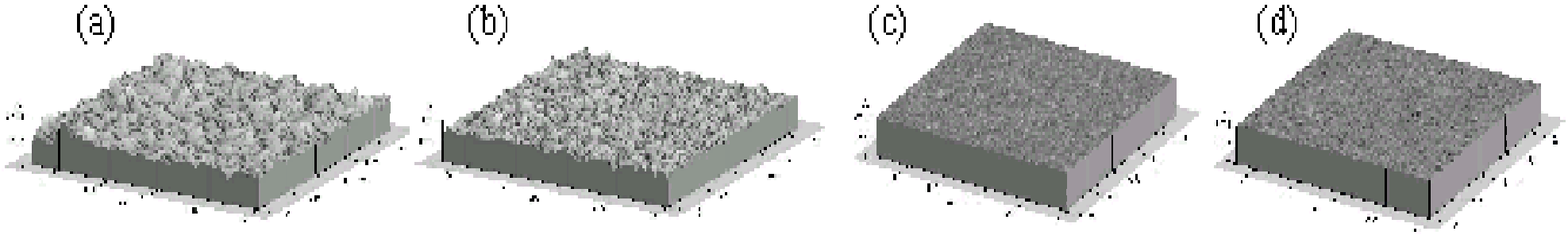
- Multiscale control objectives.
  - ◇ Reduction of film spatial nonuniformity (especially for large wafer dimensions).
  - ◇ Achievement of desired film composition and roughness.
- Estimation and control design using multiscale (deterministic / stochastic) distributed models.
  - ◇ Linking the macroscale (manipulated inputs) and microscale (control objectives).

PECVD ZrO_2 FILMS / EXPERIMENTAL RESULTS

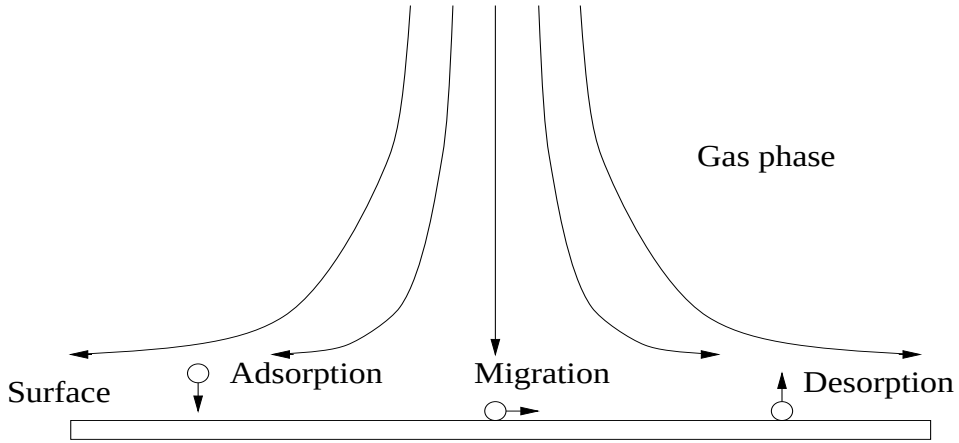
(Cho et. al, J. Appl. Phys., 2003)

- Root-mean-square (Rms) roughness decreases as the O_2/Ar flow rate ratio increases.

  Atomic force microscopy of PECVD ZrO_2 films obtained at 40 mTorr and 300 W for different O_2/Ar flow rate ratios. The measured Rms roughnesses are: (a) Rms=26.4 at O_2/Ar=0.25, (b) Rms=22.5 at O_2/Ar=0.5, (c) Rms=1.4 at O_2/Ar=1, (d) Rms=1.5 at O_2/Ar=2.0.



MULTISCALE MODELING OF THIN FILM GROWTH



- Problems due to the large disparity of time and length scales of phenomena occurring in gas phase and surface:
  - ◇ The assumption of continuum is not valid on the surface.
  - ◇ Computationally impossible to model the whole system from a molecular point of view.

- Solution to bridge the macroscopic and microscopic scales:
  - ◇ Model the continuous gas phase by PDEs.
  - ◇ Model the configuration of the surface by Monte-Carlo techniques.
  - ◇ Incorporate the results of MC simulation to PDEs via boundary conditions.

GAS PHASE MODEL

- Conservation of momentum, energy and mass in a stagnation flow geometry (Sharma, et. al. Combust. Sci. Technol., 1969):

$$\frac{\partial}{\partial \tau}(\frac{\partial f}{\partial \eta}) = \frac{\partial^3 f}{\partial \eta^3} + f\frac{\partial^2 f}{\partial \eta^2} + \frac{1}{2}[\frac{\rho_b}{\rho} - (\frac{\partial f}{\partial \eta})^2]$$
$$\frac{\partial T}{\partial \tau} = \frac{1}{P_r}\frac{\partial^2 T}{\partial \eta^2} + f\frac{\partial T}{\partial \eta}$$
$$\frac{\partial y_i}{\partial \tau} = \frac{1}{Sc_j}\frac{\partial^2 y_i}{\partial \eta^2} + f\frac{\partial y_i}{\partial \eta}$$

- Boundary conditions:

  For $(\eta \to \infty)$:

$$T = T_{bulk}, \frac{\partial f}{\partial \eta} = 1,$$
$$y_j = y_{jb}, j = 1, \ldots, N_g$$

  For $(\eta \to 0)$:

$$T = T_{surface}, f = 0, \frac{\partial f}{\partial \eta} = 0$$
$$\frac{\partial y_i}{\partial \eta} = \frac{Sc_{growing}(R_a - R_d)}{\sqrt{2a\mu_b\rho_b}}$$

SURFACE MICROSTRUCTURE MODEL

- Kinetic Monte-Carlo model:
  - ◇ First-nearest-neighbor interactions only.
  - ◇ Solid-on-solid approximation of a simple cubic lattice.
  - ◇ Adsorption, desorption and migration only.
  - ◇ Periodic boundary conditions.

- Rates of adsorption, desorption and migration:

$$r_a = \frac{s_0 P}{2a\sqrt{2\pi m k T} C_{tot}}$$

$$r_d(n) = \frac{\nu_0}{2a} exp(-\frac{nE}{kT})$$

$$r_m(n) = \frac{\nu_0 A}{2a} exp(-\frac{nE}{kT})$$

SURFACE MICROSTRUCTURE MODEL

- The life time of every MC event is determined by a random number and the total rate:

$$\Delta\tau = \frac{-\ln \xi}{r_{tot}}$$

$$r_{tot} = r_a \times N_T + \nu_0(1+A)\sum_{m=1}^{5} N_m \exp(\frac{-mE}{kT})$$

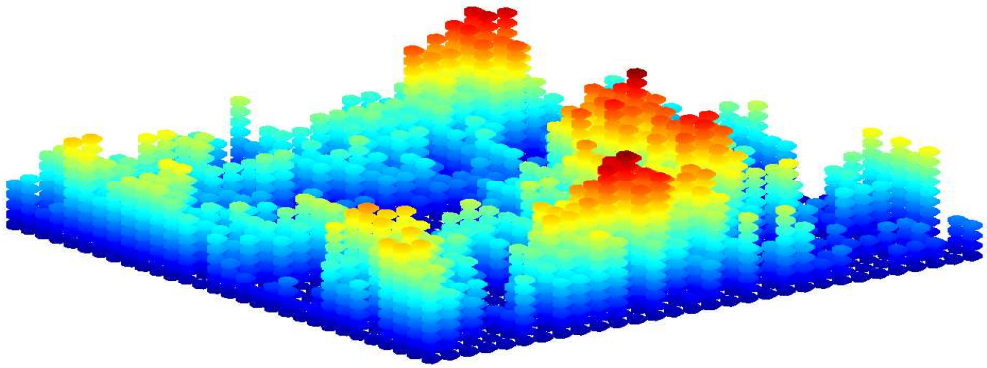
ξ: a random number in the $(0,1)$ interval.

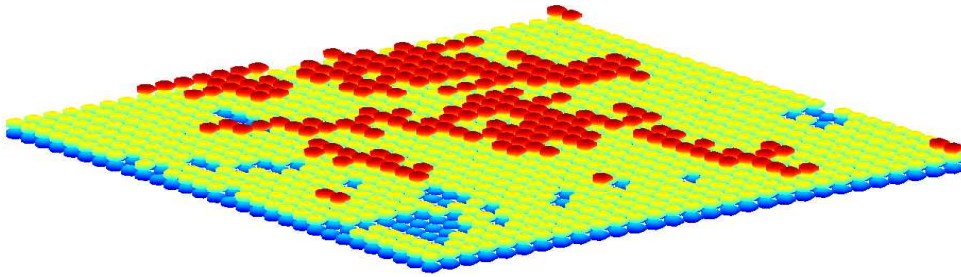
N_T: total number of sites.

N_m: number of surface atoms that have m neighbors on the surface.

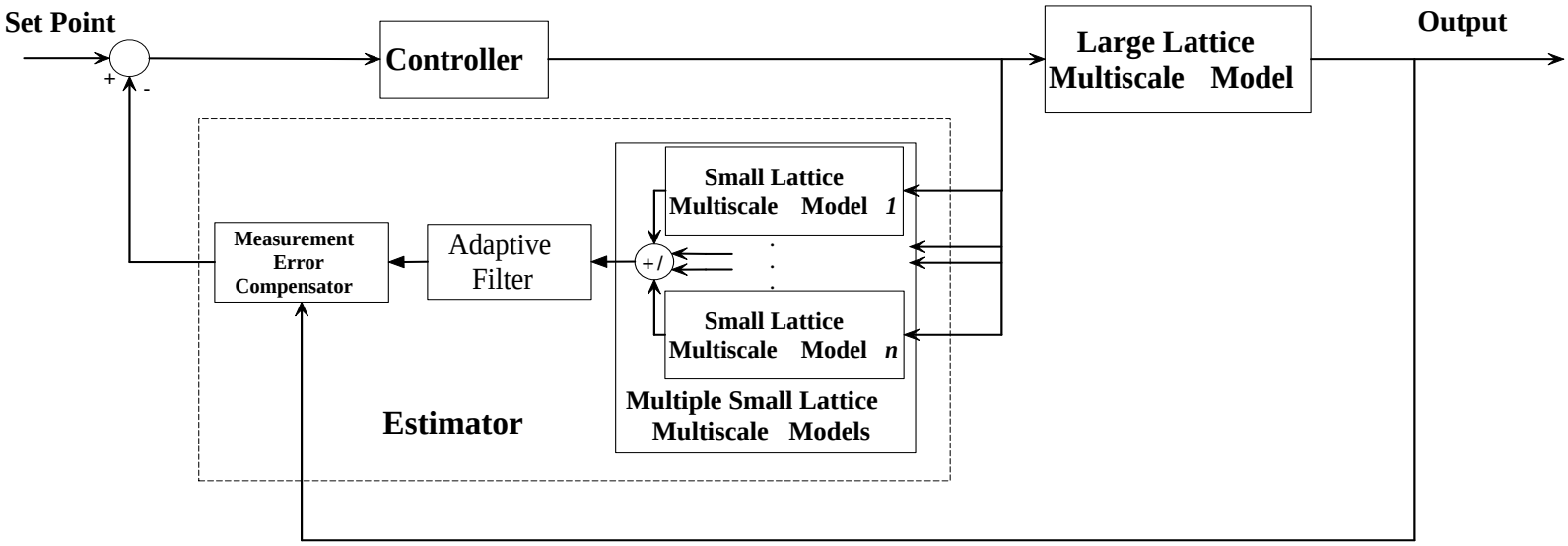
SIMULATION OF SURFACE ROUGHNESS

- Thin film microstructure and surface microprocesses.
  - ◇ Adsorption events roughen the surface.
  - ◇ Migration and desorption smoothen the surface.
- Effect of substrate temperature on surface roughness.
  - ◇ High temperature reduces surface roughness by increasing the rates of desorption and migration.
  - ◇ Left figure: configuration of film surface at T=600K.
  - ◇ Right figure: configuration of film surface at T=950K.





CONTROL PROBLEM / CONTROLLER DESIGN



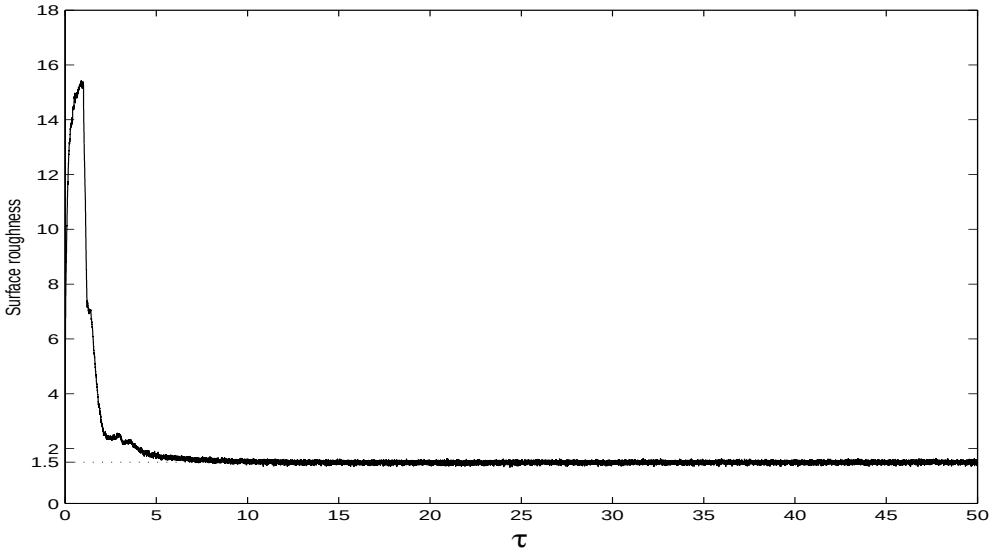
- Surface configuration/roughness is computed using a kinetic MC model that employs a large lattice.
- A feedback controller, using a roughness estimator, is used to control the surface roughness by adjusting substrate temperature.
- Roughness measurements (infrequent) can be obtained using scanning tunnelling microscopy and atomic force microscopy.

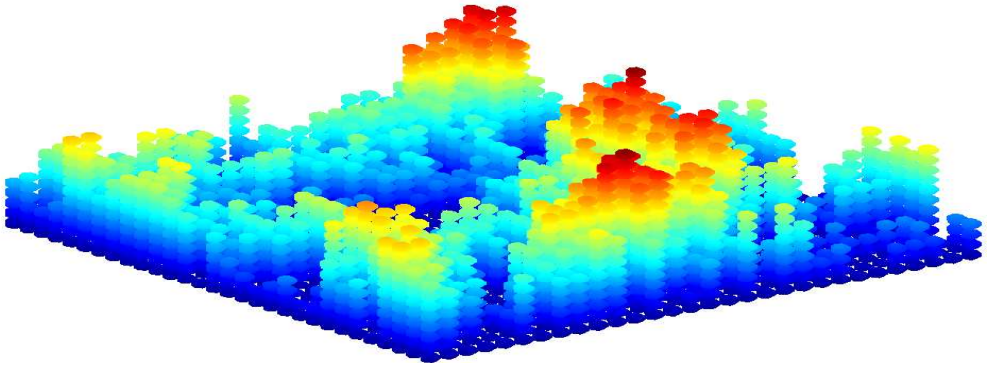
MULTISCALE CLOSED-LOOP SIMULATION RESULTS

- Initial growth at $T = 600K$.
- Initial roughness is 15.5.
- The desired roughness is 1.5.

Left figure: average surface roughness under feedback control.

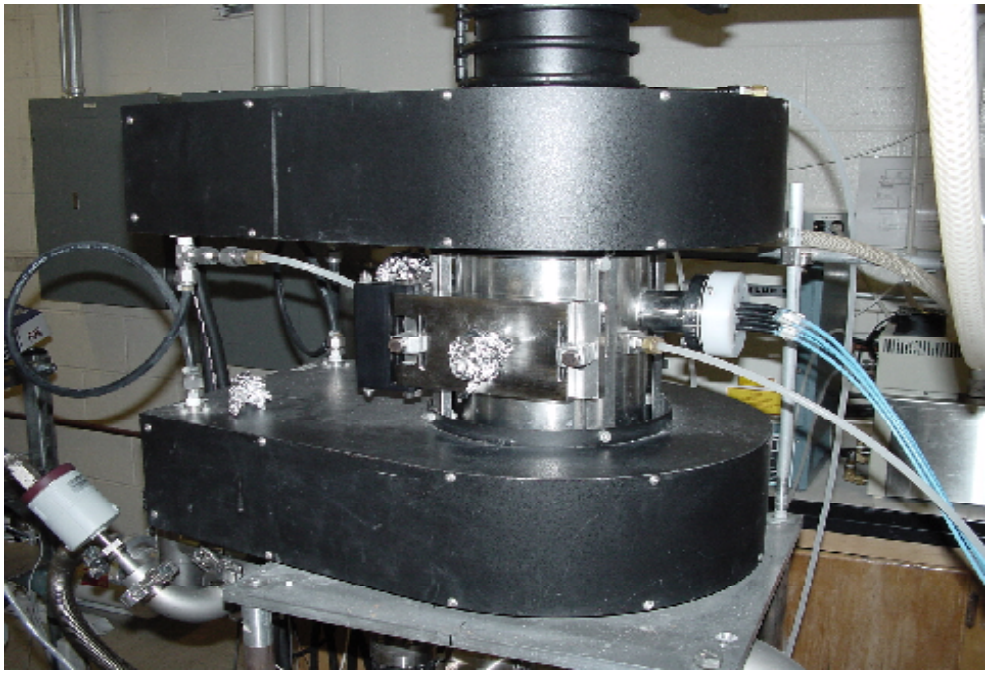
Right figure: configuration of film surface under feedback control.

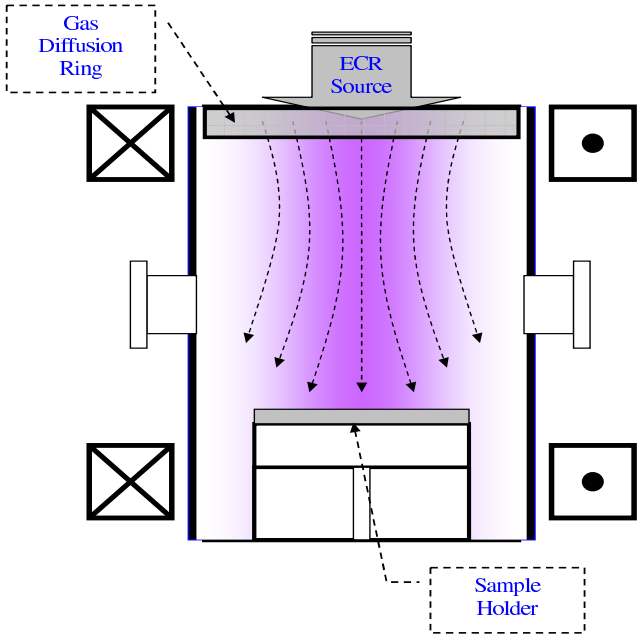




REAL-TIME CARBON CONTENT CONTROL IN PECVD

(Ni, Christofides and Chang, Proc. ACC, 2003)

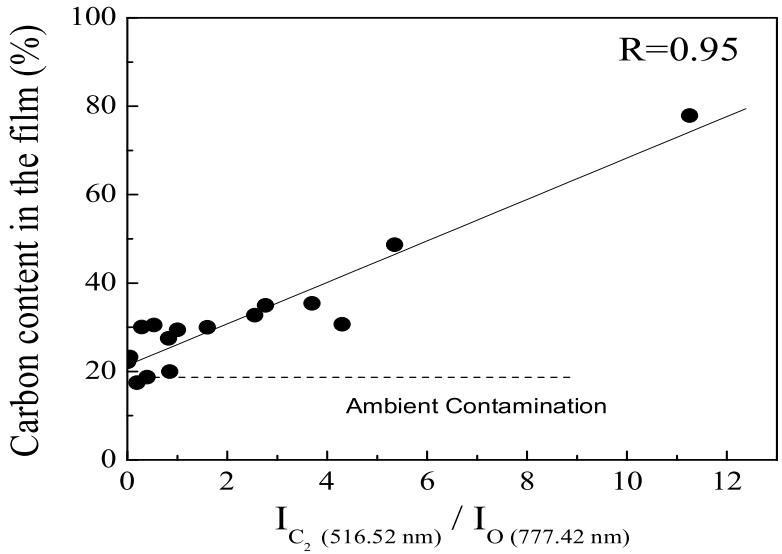




- PECVD ZrO_2 in an electron cyclotron resonance (ECR) reactor.
- Real-time carbon content estimator based on optical emission spectroscopy (OES) measurements.
- Feedback control of the carbon content in the ZrO_2 film.
  - ◇ Controller design based on the real-time carbon content estimates.
  - ◇ Control the carbon content in the film by manipulating the mass flow rate of O_2.

REAL-TIME CARBON CONTENT ESTIMATION USING OES

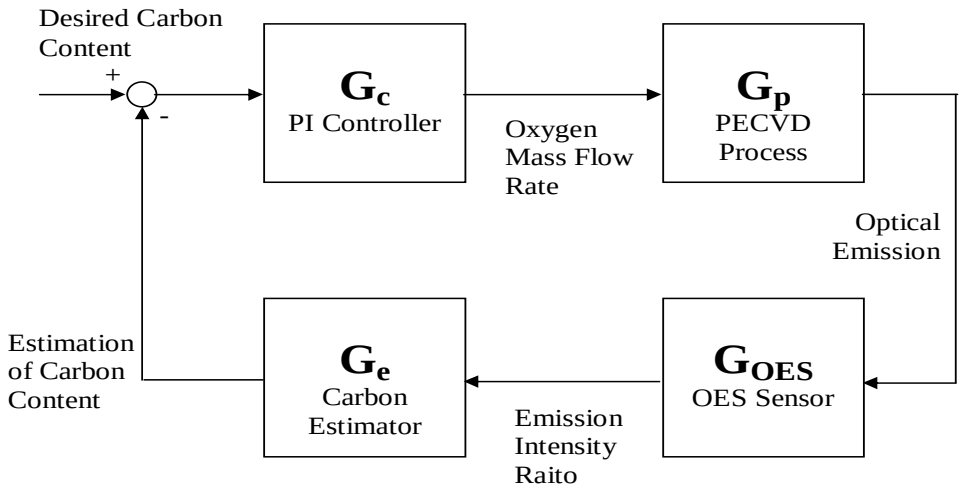
- Real-time measurements of optical emission intensity ratio of C_2 and O from OES.
- Correlation of carbon content with optical emission intensity ratio of C_2 and O obtained from XPS measurements (Cho et al., 2001).



- Real-time carbon content estimation model:

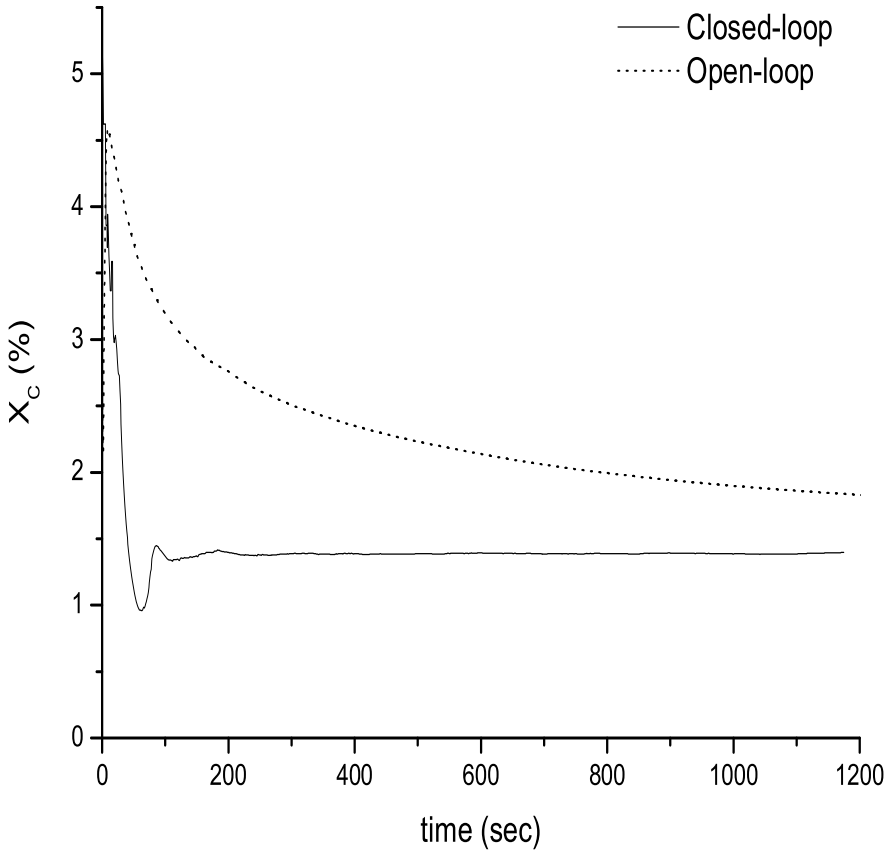
$$N(k) = \frac{4.69}{k - k_0}\gamma(k) + N(k-1)\frac{k - k_0 - 1}{k - k_0} \qquad k > k_0$$

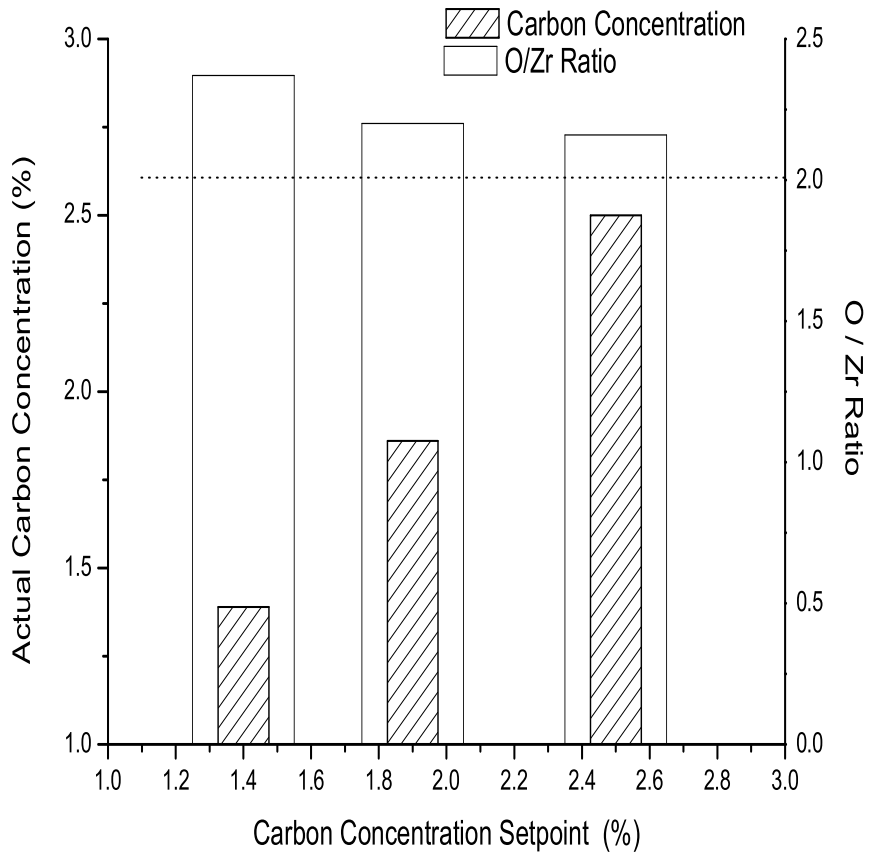
REAL-TIME CARBON CONTENT CONTROL SYSTEM



- Carbon content was estimated from OES measurement of intensity ratio of C_2 and O in real-time.
- Control the carbon content to desired level by manipulating the O_2 mass flow rate.
- The control problem is formulated as a set-point regulation problem.
  - ◇ Response time of the closed-loop system is significantly smaller than the total deposition time.

EXPERIMENTAL RESULTS OF CLOSED-LOOP SYSTEM





- Film carbon content is controlled at the desired values (verification via XPS).
- Film carbon content is significantly reduced under feedback control.

SUMMARY

- Methods for nonlinear order reduction and control
  for various classes of nonlinear distributed parameter systems.
  - ◇ Galerkin's method - approximate inertial manifold.
  - ◇ Control design using geometric and Lyapunov techniques.
  - ◇ Control using MC models.
- Applications to complex distributed processes.
  - ◇ Temperature profile / roughness / composition control in CVD.
  - ◇ Temperature / thermal gradient control in crystal growth.
  - ◇ Control of size distribution in crystallization.
- Research challenges (Christofides, AIChE J. (Perspective), 2001).

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- Former graduate students: Charalambos Antoniades, Antonios Armaou, James Baker, Eugene Bendersky, Timothy Chiu, and Ashish Kalani.

- Current doctoral students: Nael El-Farra, Stevan Dubljevic, Mingheng Li, Yiming Lou, Prashant Mhaskar, Dong Ni, Prasenjit Ray, Dan Shi and Adiwinata Gani.

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