Spatially Controllable CVD: The Programmable Reactor Concept

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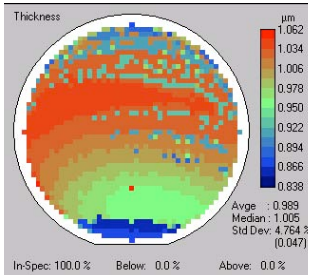
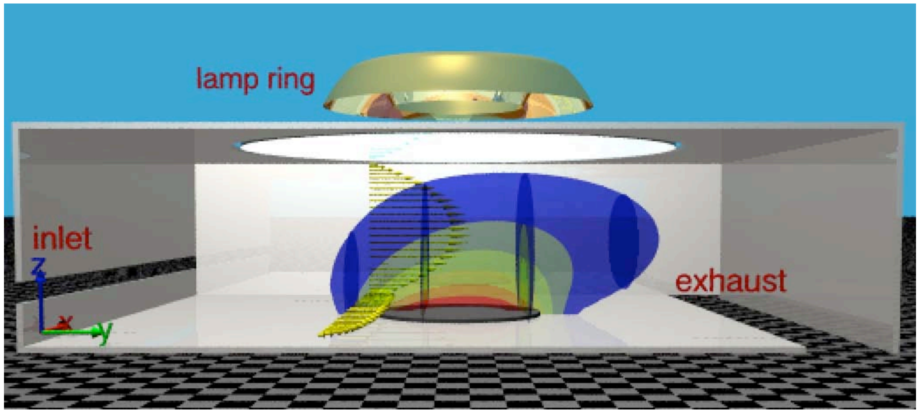
Limits of conventional CVD designs

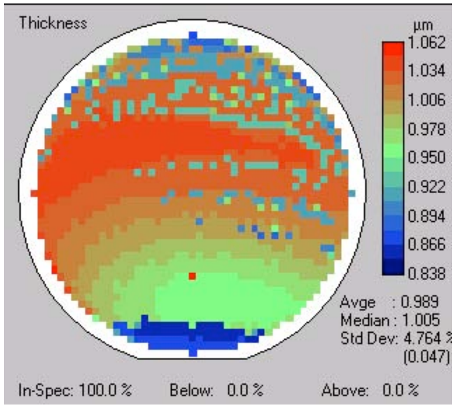


- •Inflexible
- •Process throughput / uniformity trade-offs
- •Few control inputs
- •Limited wafer access and few sensors

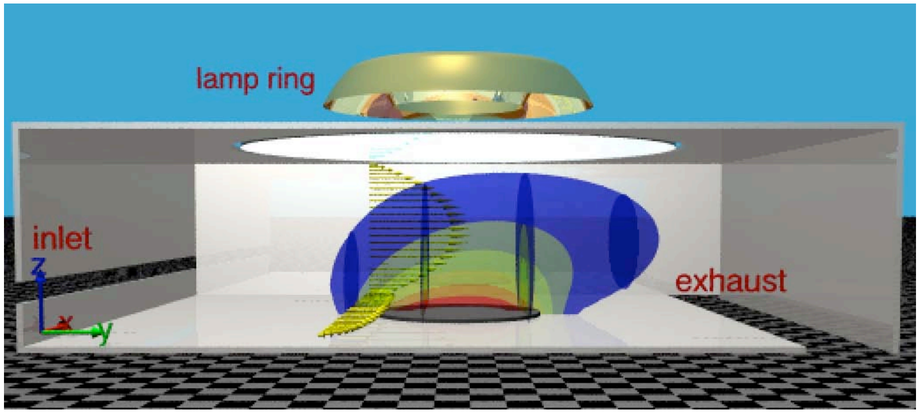


Iterative design/optimization cycle

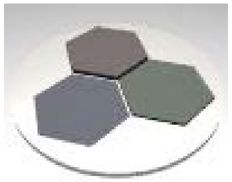
CVD process operations leading to spatially non-uniform film growth



Simulation-based assessment of design and operation alternatives



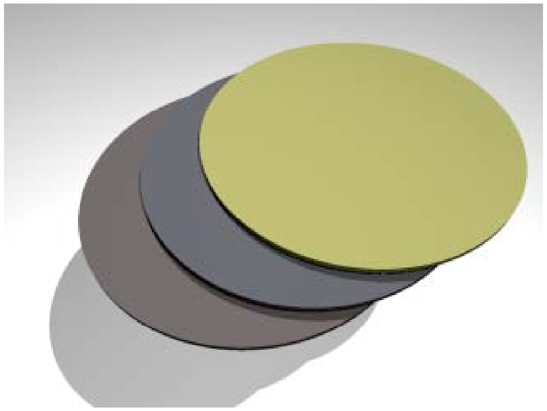
Object-oriented CVD simulation tools for diagnosing factors responsible for non-uniformity



The Programmable Reactor concept

- To achieve true 2D control of reactant gas composition across the wafer surface
- To enable single wafer combinatorial experiments for process and materials discovery
- Subsequently reprogrammable for across-wafer uniformity

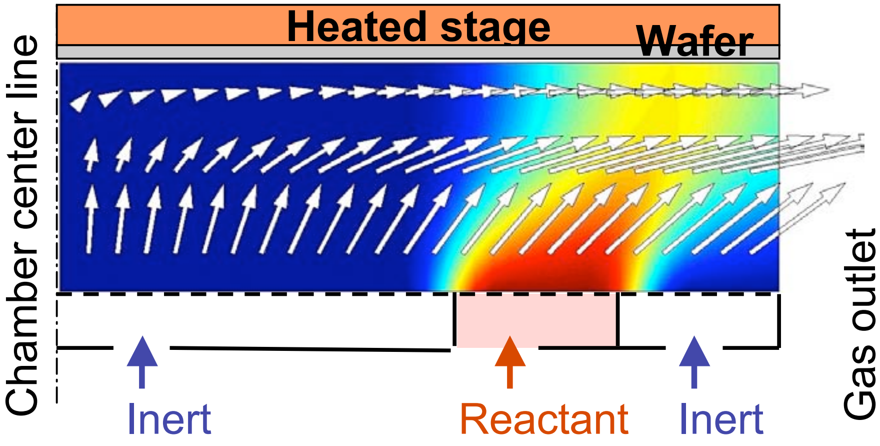
Library wafer: programmed nonuniformity



Uniform deposition at specified conditions

Previous efforts at gas composition control

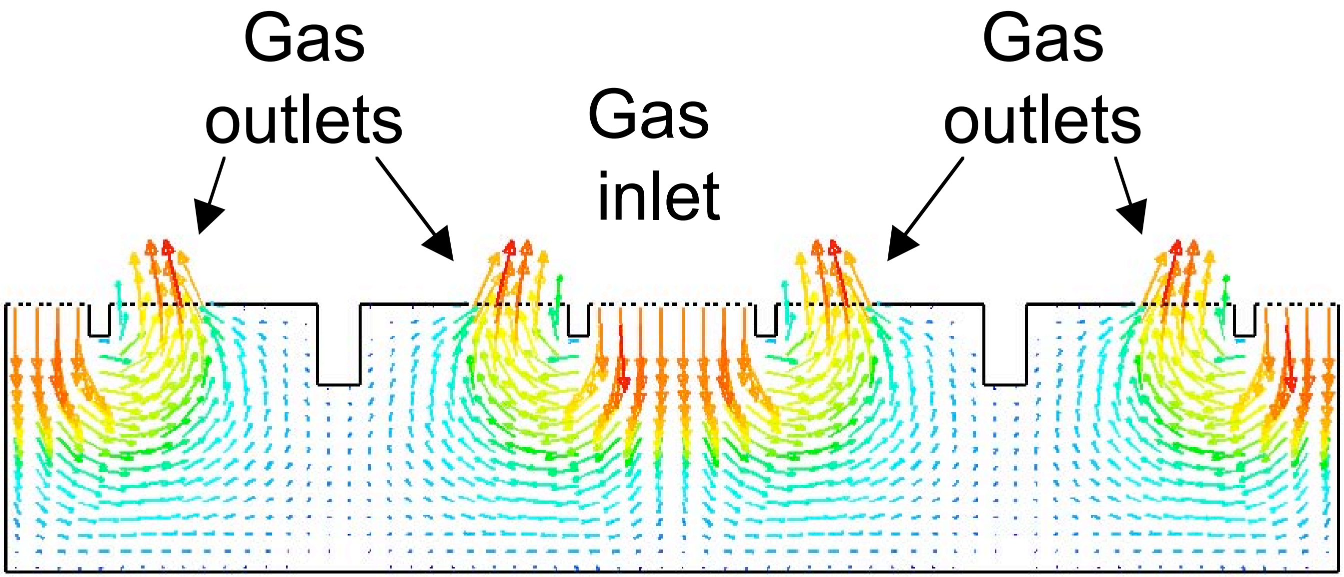
Authors	Design innovation	Material system
Moslehi, Davis, Matthews (1995)	3 annular zone showerhead	W CVD
Van der Stricht, Moerman, Demeester, Crawley, Thruch (1997)	Separate TMG, NH3 injection to reduce gas phase reactions	GaN MOCVD
Theodoropoulos, Mountziaris, Moffat, Han, Shadid, Thrush (2000)	Annual ring showerhead with alternating TMG, NH3 inlet rings	GaN MOCVD
Wang, Wang, Mahanty, Komatsu, Inaoka, Nishino, Sakai (2000)	Stacked gas delivery system with inert flow forcing reactants to wafer	GaN MOCVD



Annular-segmented showerhead gas inlets

- Designs above exhaust in "conventional" ways
- Segmented designs are subject to considerable inter-segment convective transport

Recirculating showerhead design

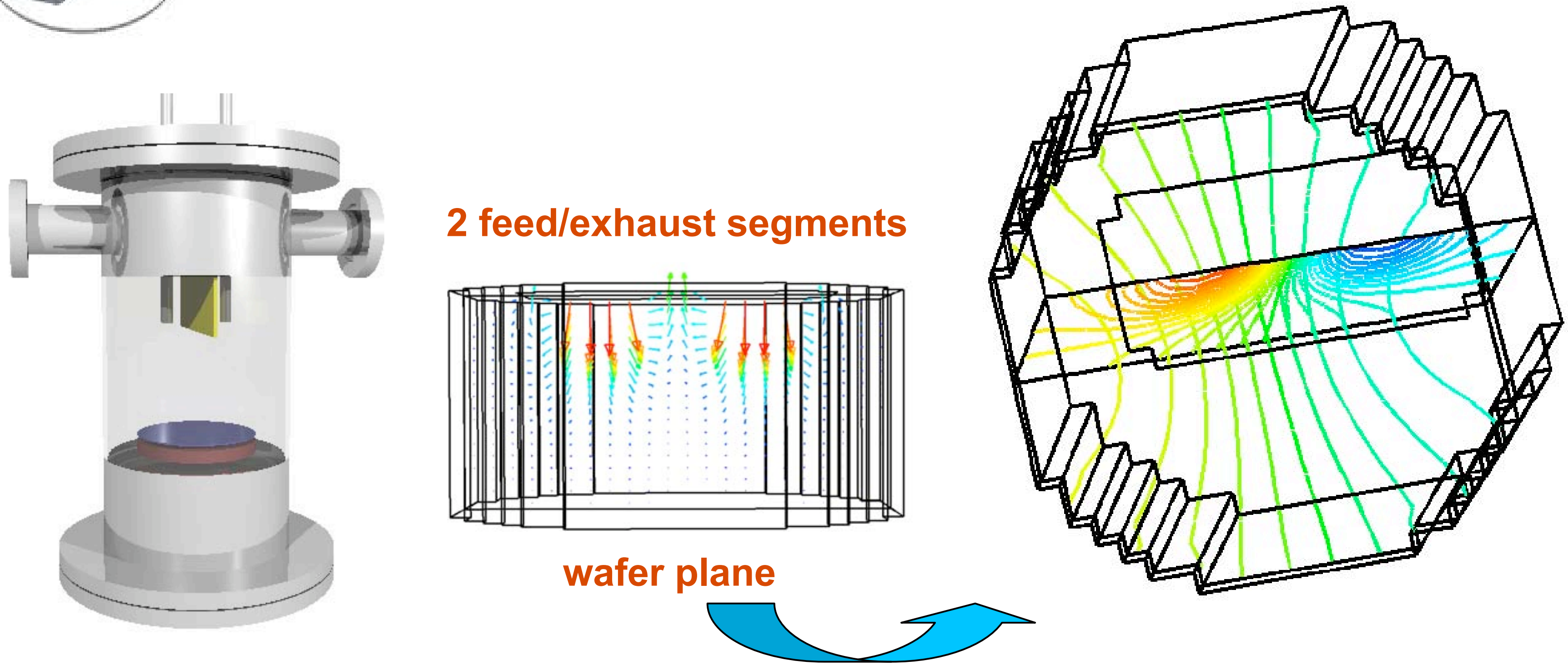


- Residual gas drawn back up through showerhead

- Periodic gas flow fields minimize inter-segment convective transport

- Residual gas can be sampled from each segment, simplifying spatial composition measurements

Control of gas composition gradients



- Inter-segment region mass transfer is governed by diffusion
- Composition gradients are controlled by
  1. Feed composition to each segment
  2. Showerhead/wafer spacing

Design of the 3-zone prototype

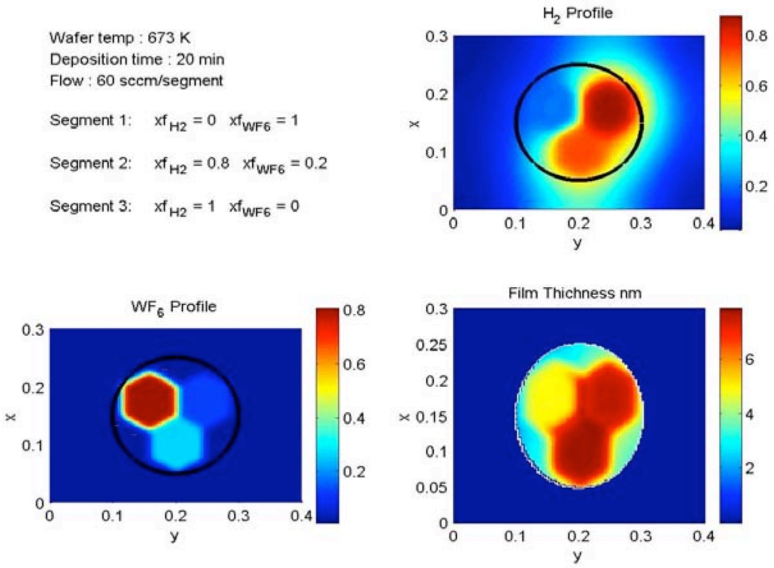
Test System:
H_2 reduction of WF_6

Wafer temp : 673 K
Deposition time : 20 min
Flow : 60 sccm/segment

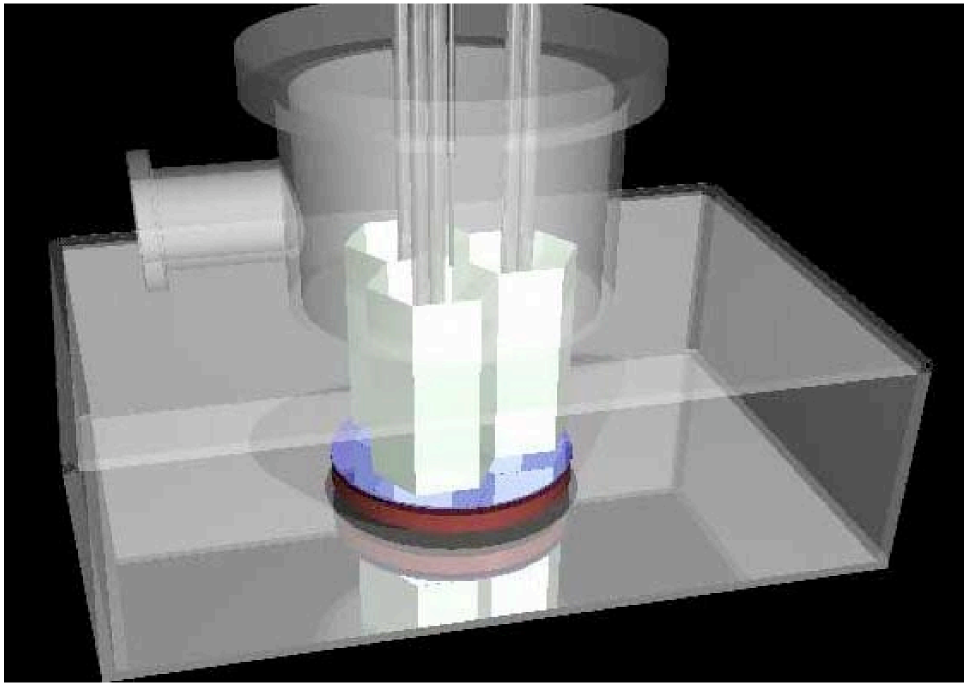
Segment 1: $xf_{H2} = 0$ $xf_{WF6} = 1$

Segment 2: $xf_{H2} = 0.8$ $xf_{WF6} = 0.2$

Segment 3: $xf_{H2} = 1$ $xf_{WF6} = 0$

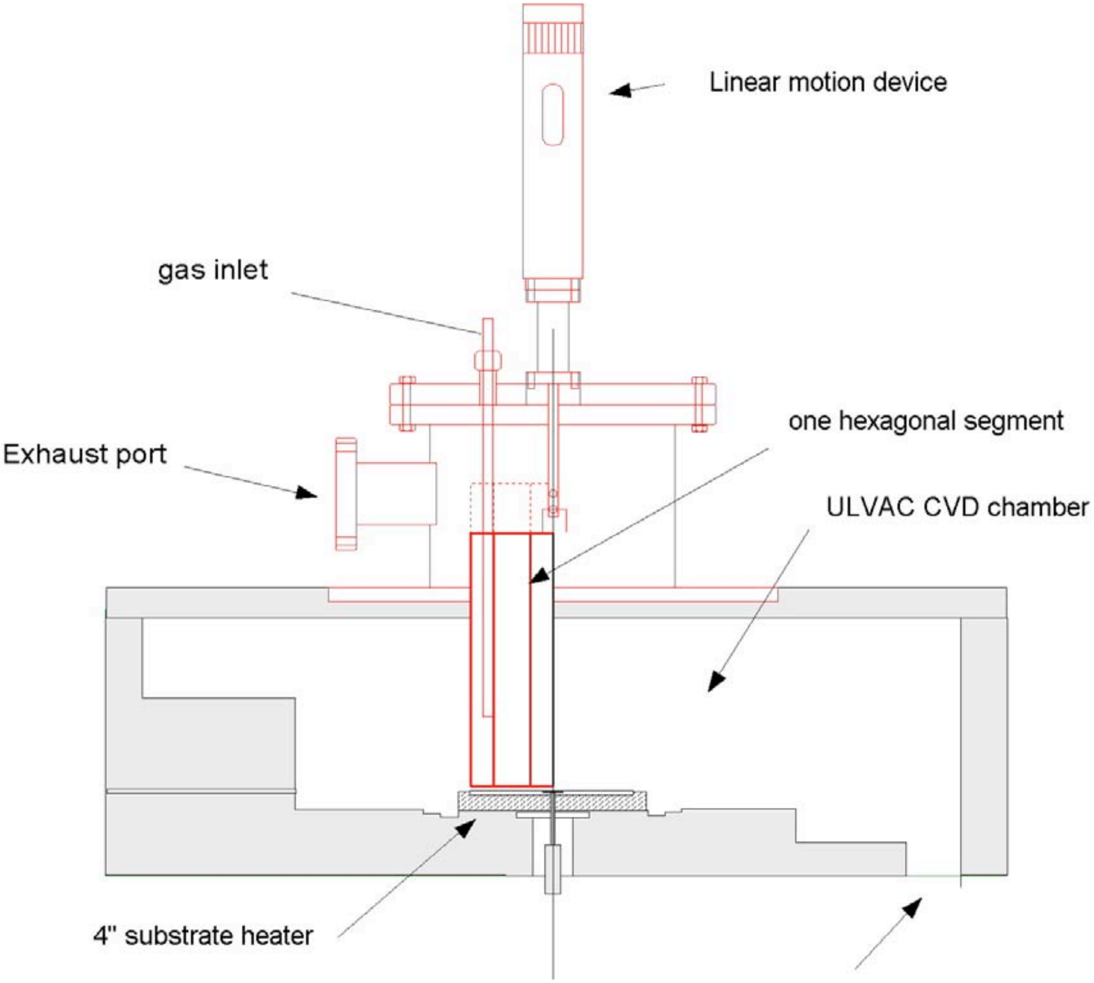


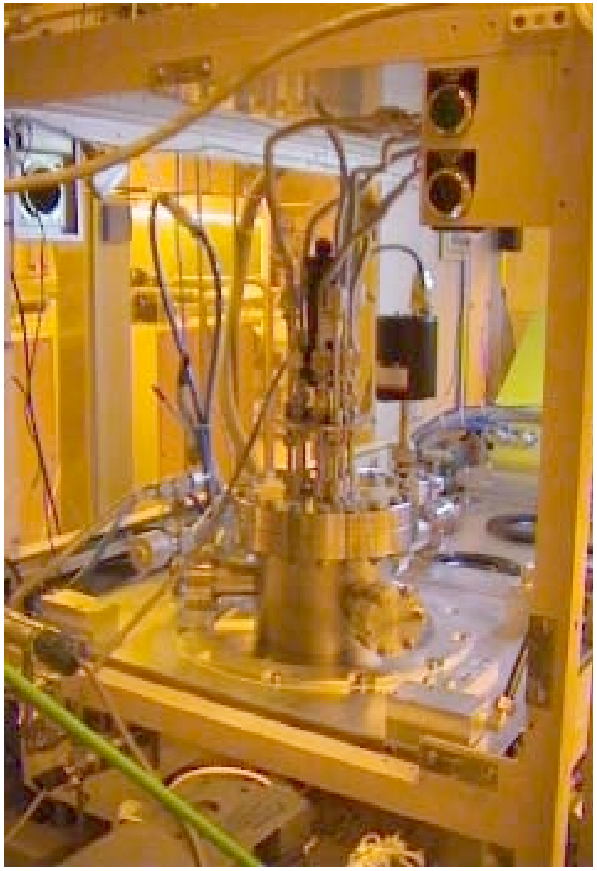
Early simulation of 2D diffusive transport in gap region for W CVD



ULVAC vacuum chamber modified for 3-segment prototype

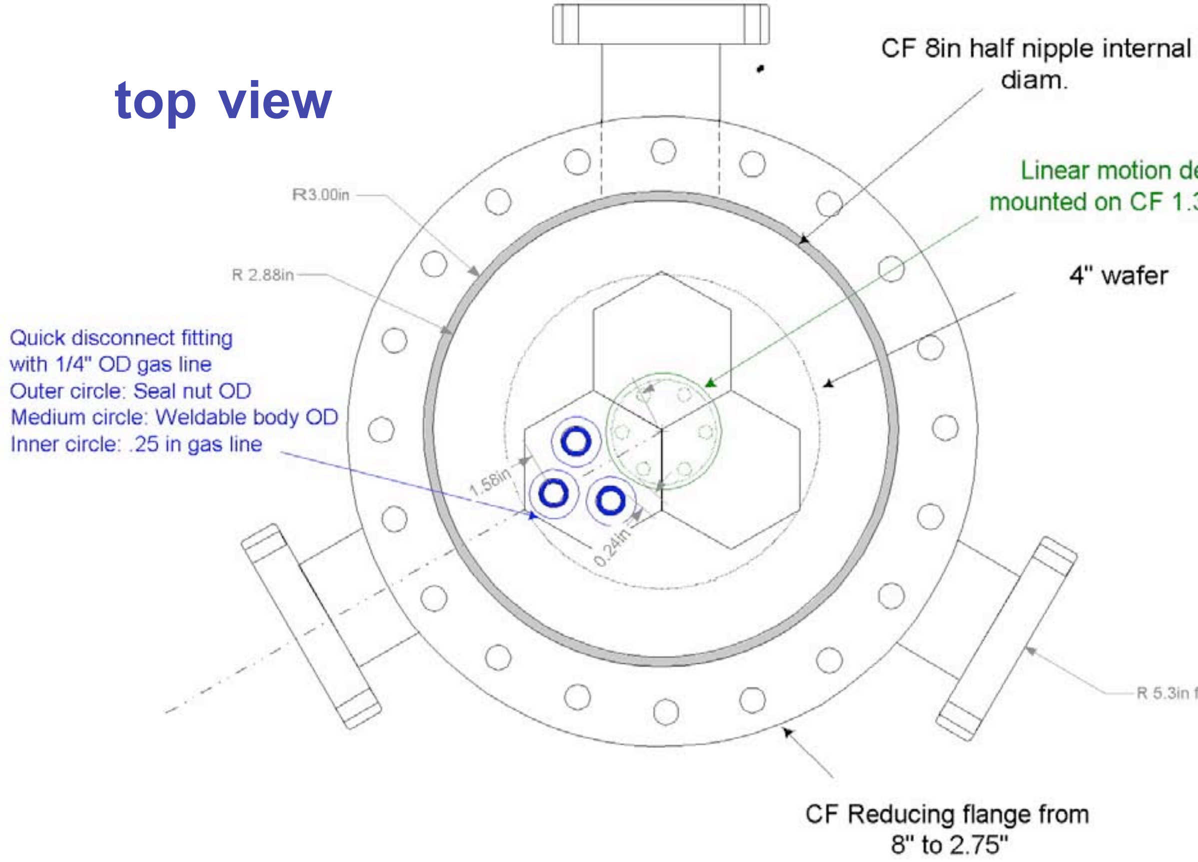
Prototype construction

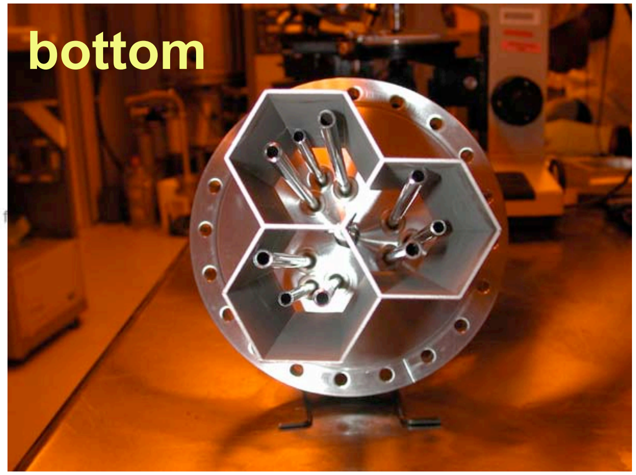




Prototype construction

top view

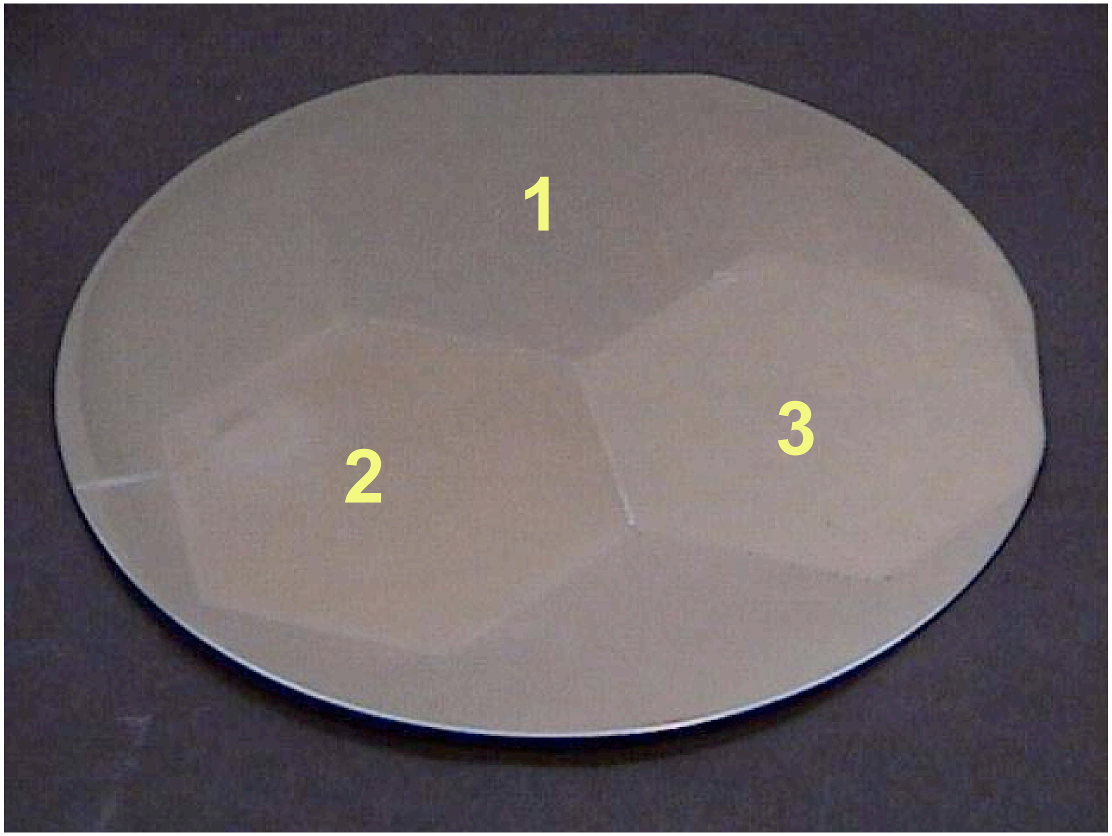




Initial experimental testing

- 3-zone prototype has been running since summer 2002
- First films deposited have demonstrated that spatially patterned wafers can be produced by controlling gas phase composition

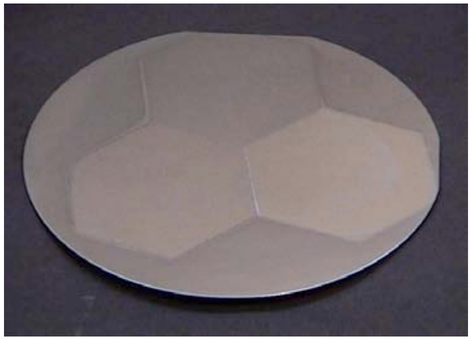
Seg 1	50 sccm Ar
Seg 2	50 sccm WF_6
Seg 3	50 sccm H_2
0.5 torr	300-350 C



Question: Why does W deposition occur in segments 1 (Ar) and 3 (H_2)?

Experimental data hierarchical structure

Wafer number: w100102-03



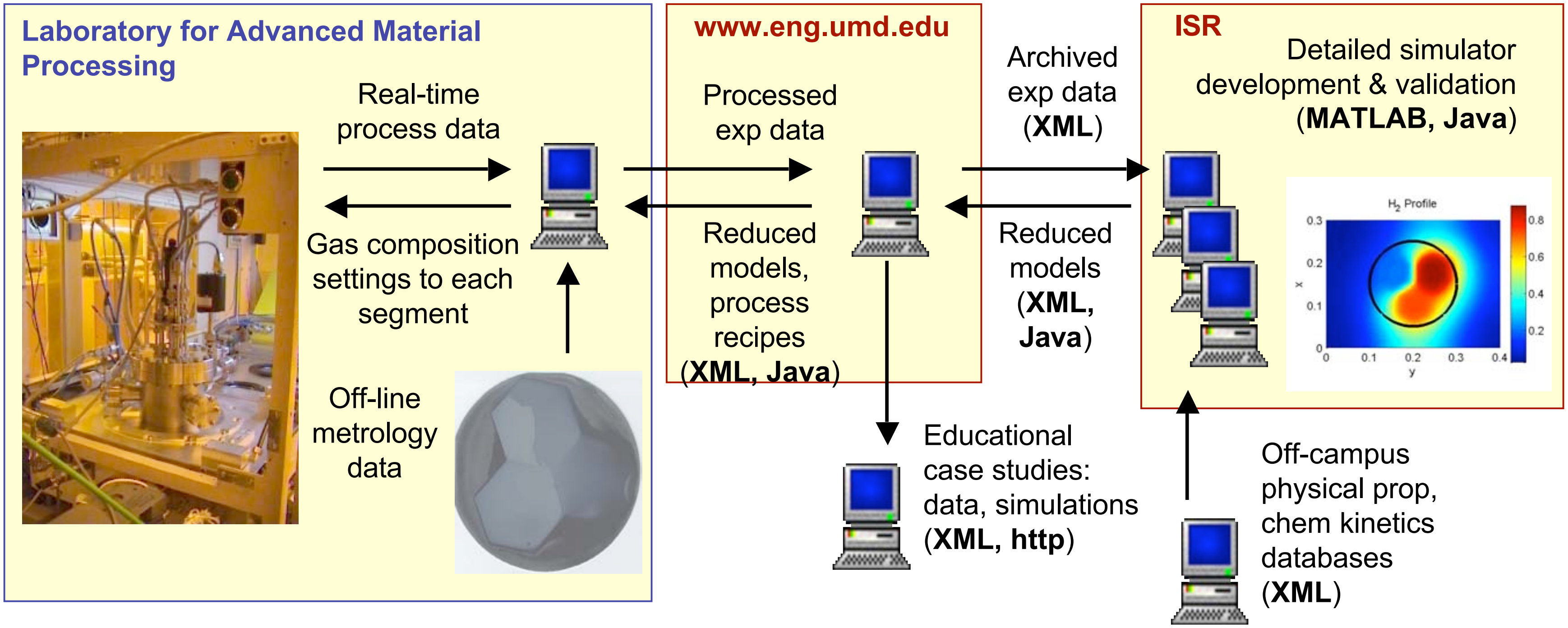
- **EquipmentData** ***(process diagnosis)***
  - **Gas line pressure**
  - **Wafer position**

- **OperatingConditions data** ***(simulator input)***
  - **Wafer/segment spacing**
  - **Segment gas flows**

- **Measurements data** ***(analysis, simulator validation)***
  - **Initial wafer mass**
  - **Final wafer mass**
  - **Sheet resistance profiles**

- **Structure influenced by use**
- **Store raw data only**

IT and distributed simulation framework



Laboratory for Advanced Material Processing

Real-time process data

Gas composition settings to each segment

Off-line metrology data

www.eng.umd.edu

Processed exp data

Reduced models, process recipes (**XML, Java**)

Archived exp data (**XML**)

Reduced models (**XML, Java**)

ISR

Detailed simulator development & validation (**MATLAB, Java**)

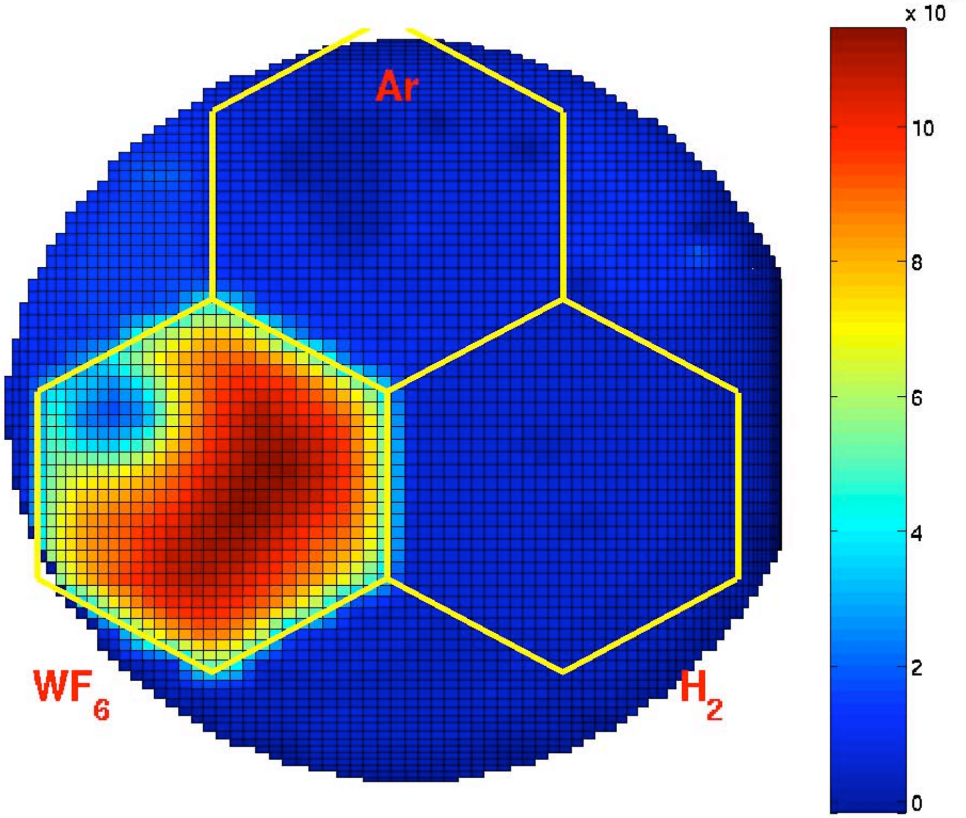
Educational case studies: data, simulations (**XML, http**)

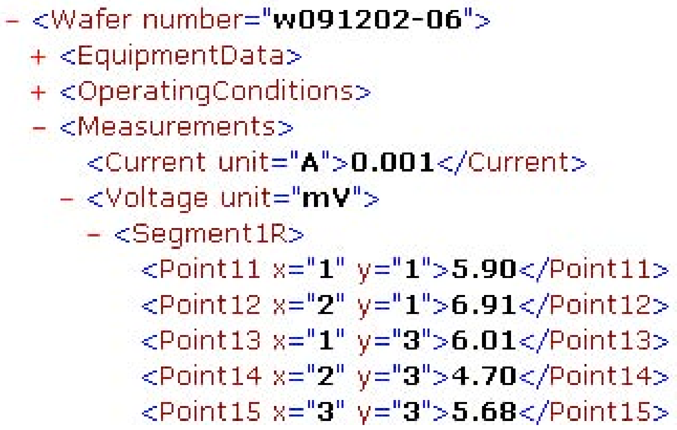
Off-campus physical prop, chem kinetics databases (**XML**)

1. Represent data in XML
2. Java parser methods called from MATLAB applications

4-point probe data analysis

W thickness map

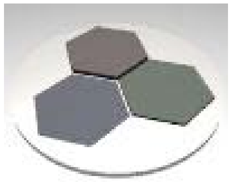




```
- <Wafer number="w091202-06">
  + <EquipmentData>
  + <OperatingConditions>
  - <Measurements>
      <Current unit="A">0.001</Current>
    - <Voltage unit="mV">
      - <Segment1R>
          <Point11 x="1" y="1">5.90</Point11>
          <Point12 x="2" y="1">6.91</Point12>
          <Point13 x="1" y="3">6.01</Point13>
          <Point14 x="2" y="3">4.70</Point14>
          <Point15 x="3" y="3">5.68</Point15>
```

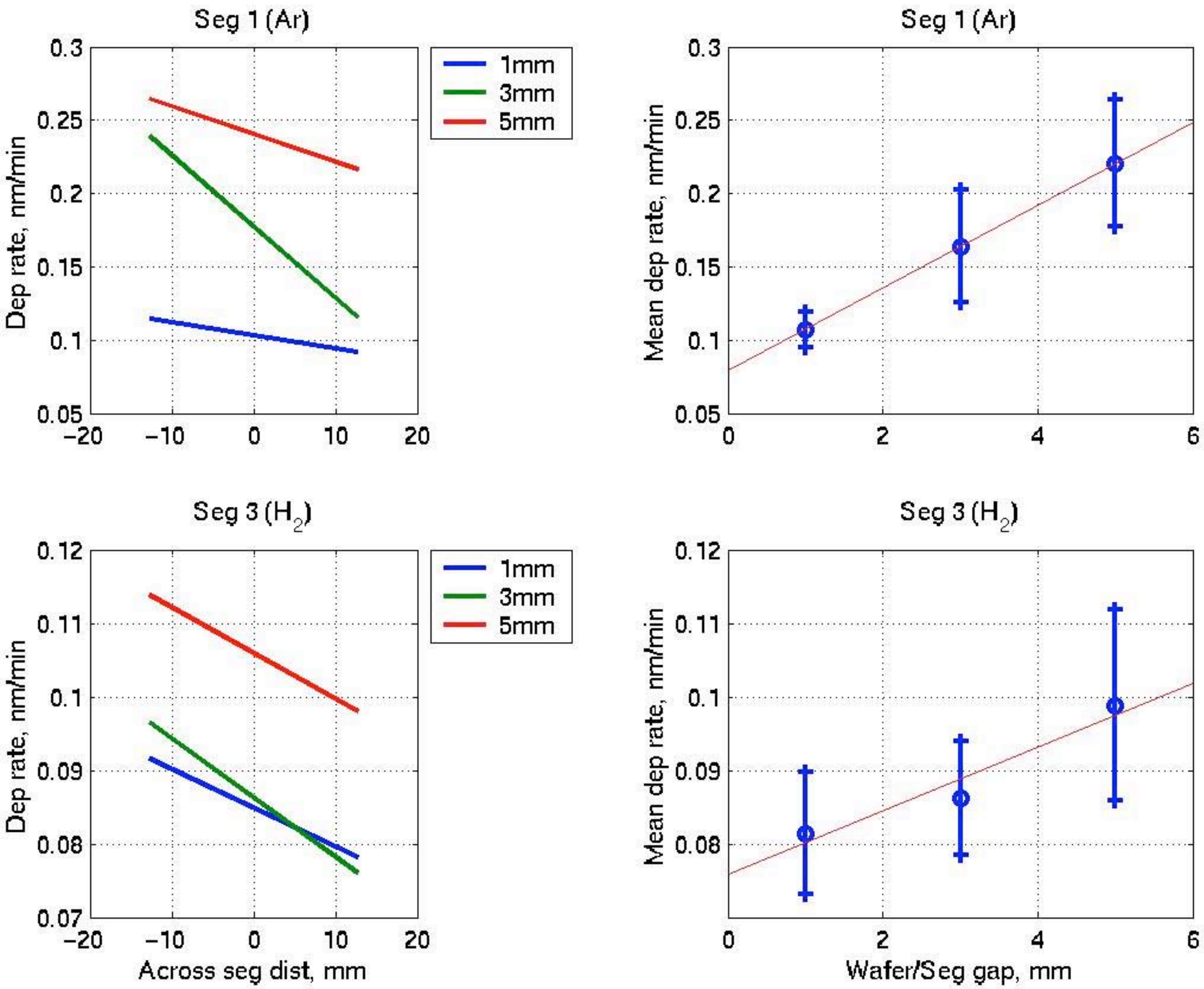
Observations

- Metrology data confirms existence of W films in Ar and H_2 segments
- Negative thickness gradient with respect to distance from WF_6 segment
- Thickness in Ar and H_2 segments grows with gap



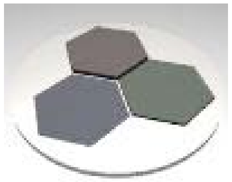
W deposition profiles

Deposition Rate

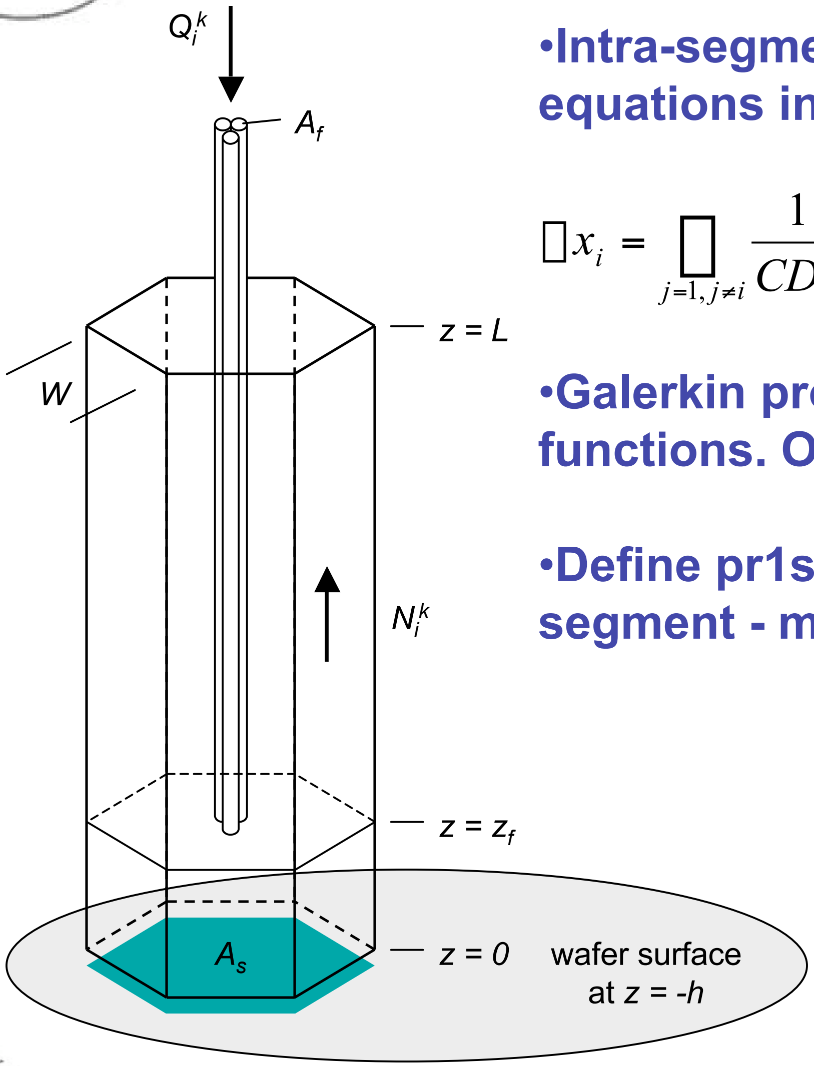


Dist from WF_6 Seg →

Gap size →



Segment transport model



- **Intra-segment transport model: Stefan-Maxwell equations including thermal diffusion;**

$$\nabla x_i = \sum_{j=1, j\neq i} \frac{1}{CD_{ij}}\left(x_i \overline{N}_j - x_j \overline{N}_i\right) \quad \overline{N}_i = N_i + \frac{\mathbf{D}_i^T}{M_i}\nabla \ln T$$

- **Galerkin projection solution on global basis functions. Outlet BC: exhaust volume model;**

- **Define pr1seg class objects to model *each* segment - modularity;**

- **Define wafer/showerhead gap region inter-segment diffusion model object;**

- **Download operating conditions from data archive website to define objects.**

Object-oriented MWR

Benefits to hiding details of computations:

1) Clear connection between modeling equations and solution procedure

2) One-to-one correspondence between computational tools and steps to implement MWR

Model

$$\begin{aligned} \frac{\partial T}{\partial t} &= \nabla^2 T - v_x \frac{\partial T}{\partial x} + R_c(T) \\ T(x,y,t) &= \sum_{i=1}^{M} \sum_{j=1}^{N} a_{i,j}(t)\phi_i(x)\psi_j(y) \end{aligned}$$

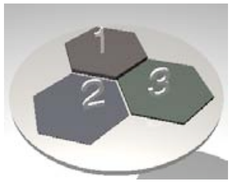
$$\begin{aligned} \mathrm{F.val} &: \{\phi\ , \psi\ \} \\ \mathrm{F.dir} &: [1,2] \\ \mathrm{F.wt} &: \{\mathbf{w_x}, \mathbf{w_y}\} \end{aligned}$$

Basis function object

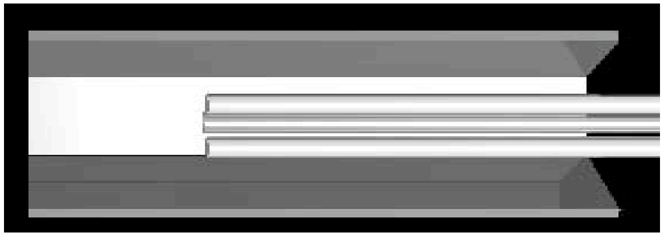
Overloaded operators and functions

$$\begin{aligned} \mathbf{T} &= \mathbf{a} * \mathrm{F} \\ \dot{\mathbf{a}} &= \mathtt{wip}(\mathbf{DDX} * \mathbf{T} + \mathbf{DDY} * \mathbf{T} - \mathbf{v_x} * \mathbf{DX} * \mathbf{T} + \mathbf{R_c}, \mathrm{F}) \end{aligned}$$

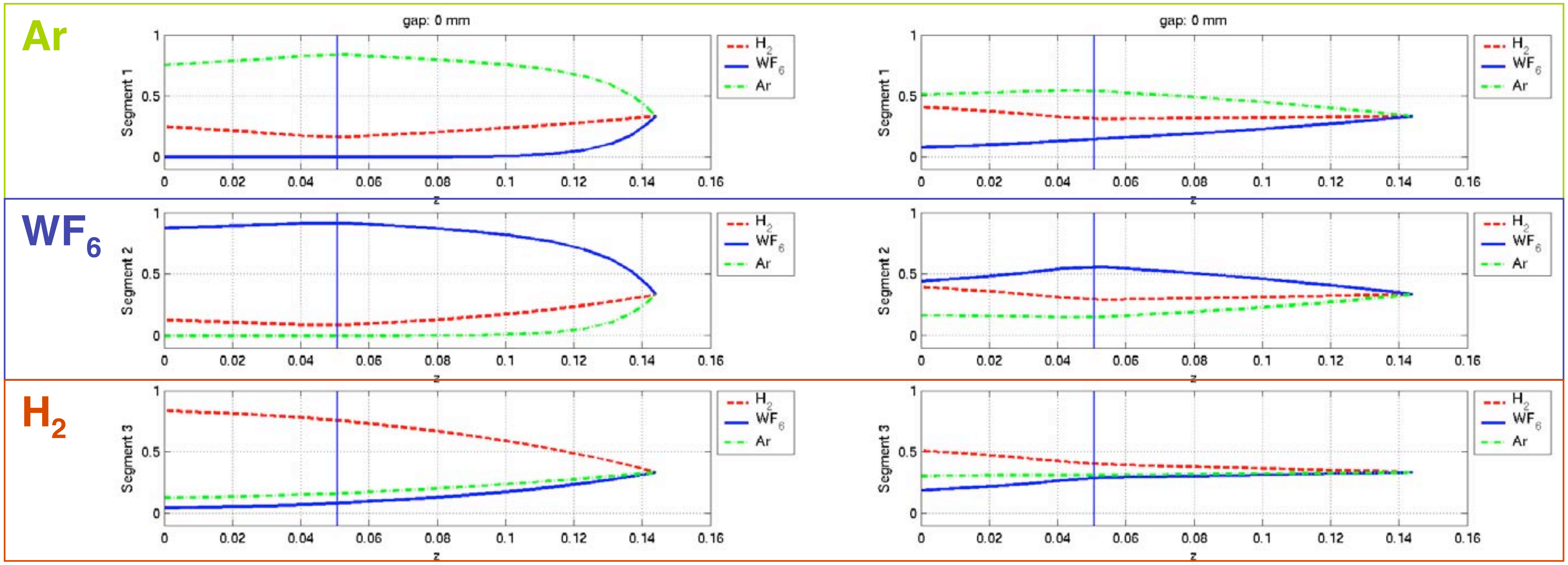
Adomaitis, Comp & ChE, 2002



Segment gas composition profiles



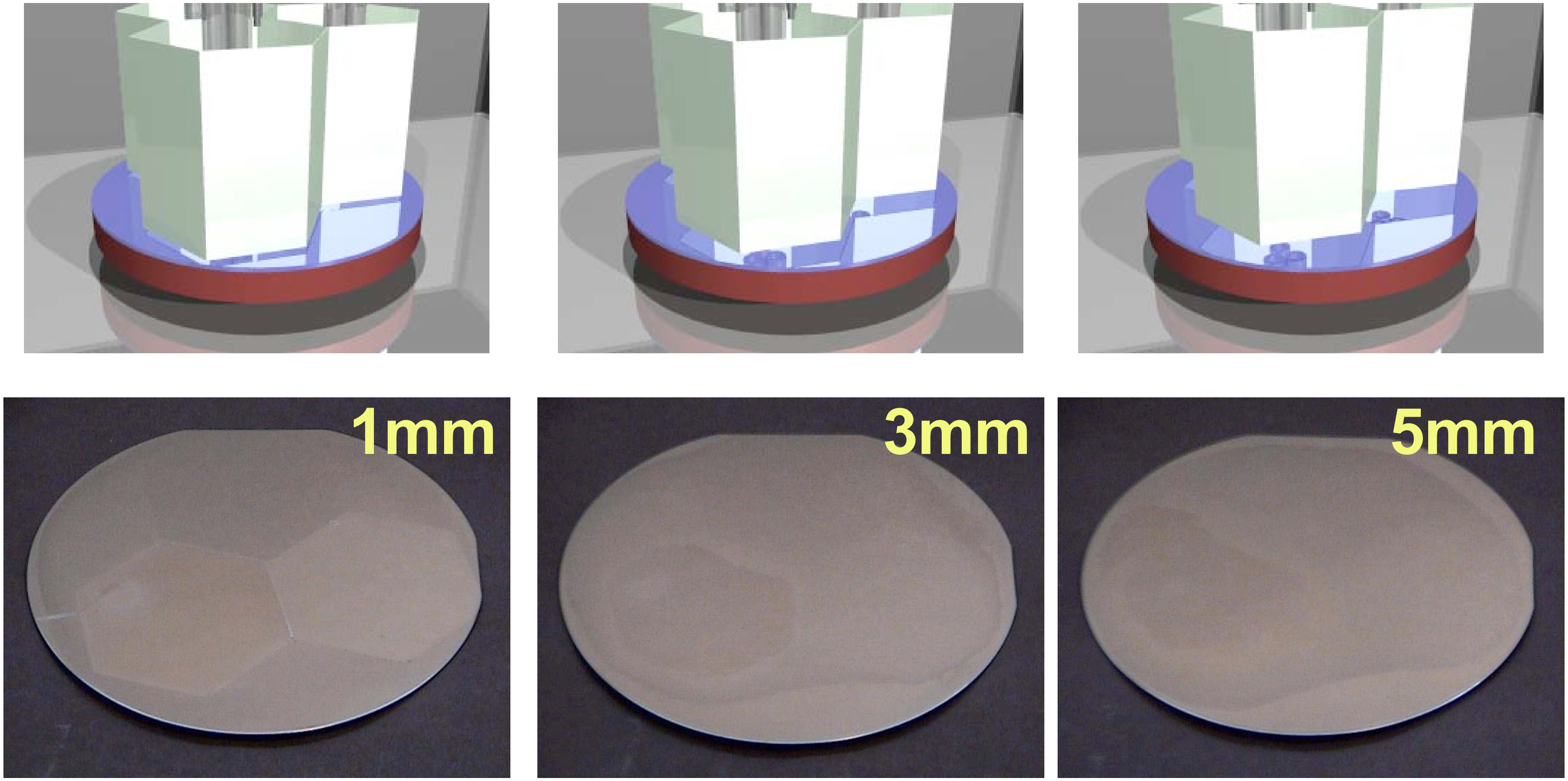
- Close wafer/showerhead spacing
- Significant effect of feed gas flow
- Thermal diffusion effects
- Back-diffusion from common exhaust region to wafer surface



50 sccm / segment

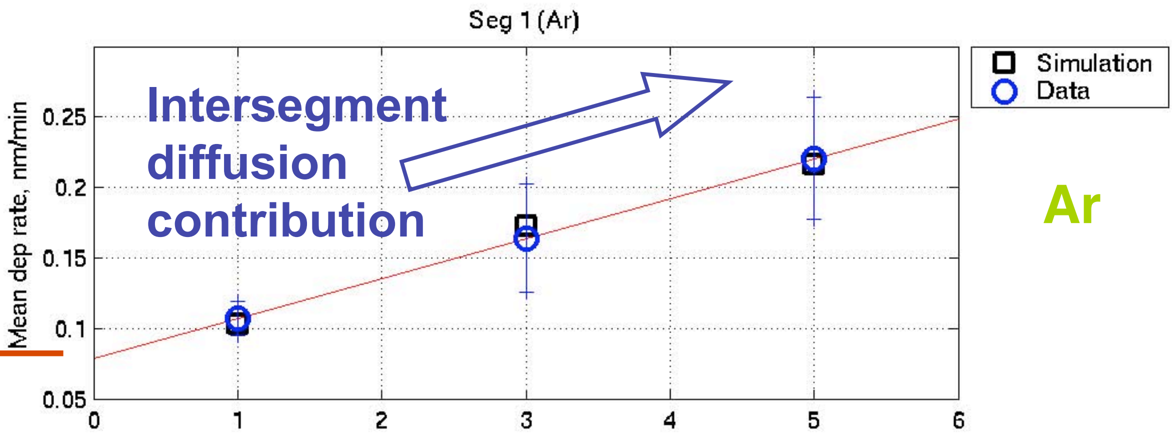
5 sccm / segment

Deposition pattern control



Increasing across-wafer diffusion

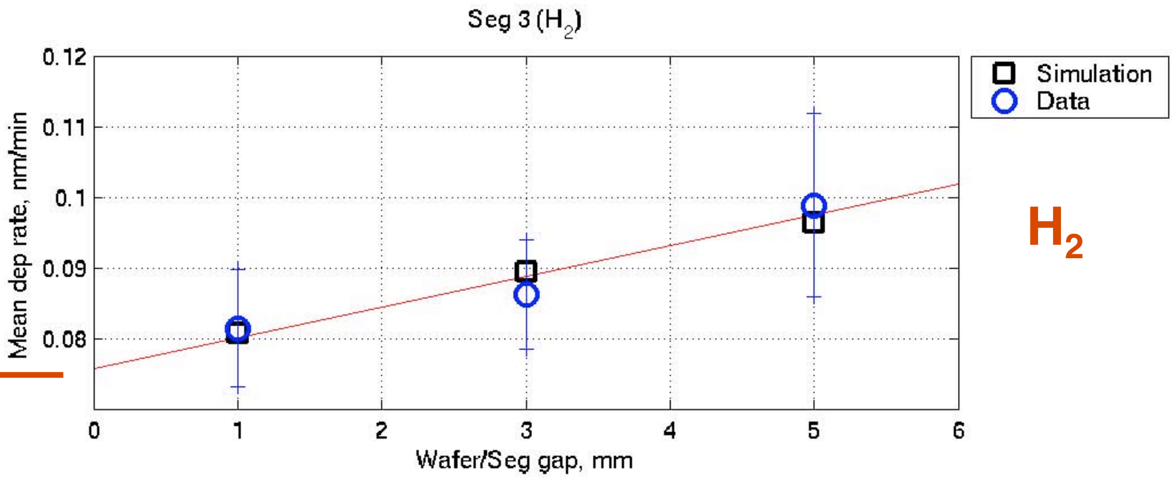
Effect of gap size on film thickness



Intersegment diffusion contribution

Ar

Back diffusion contribution

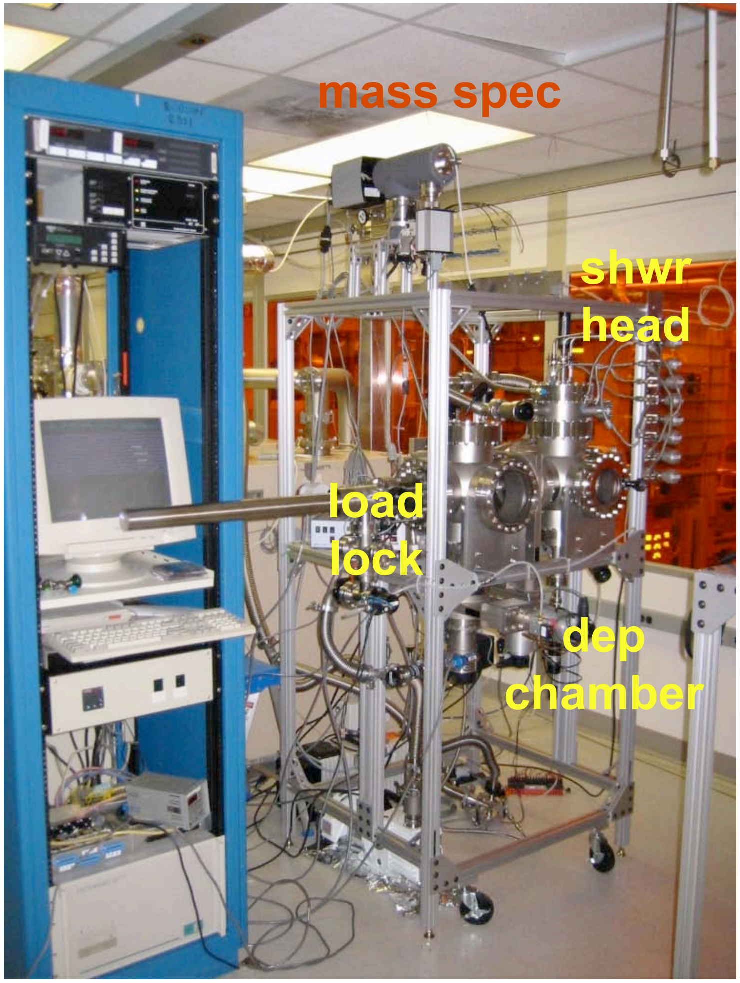


H_2

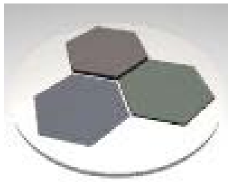
Back diffusion contribution

Gap size

Current Programmable Reactor research



- Complete reconstruction of 3-zone prototype to improve reliability and achieve true programmability;
- Simulation-based design of next generation reactor: more segments per showerhead; smaller segments incorporating micro-fabricated flow control; improved manufacturability.



Conclusions

- A new approach to spatially controllable CVD was presented; reactor featured a reverse-flow, segmented showerhead design;
- Gas composition to each segment can be controlled and sampled;
- Gas composition at wafer surface is governed intra-segment back diffusion (controlled by gas feed rate) and across wafer inter-segment diffusion (controlled by wafer/showerhead gap size);
- 3 zone prototype was constructed; initial testing demonstrated the feasibility of spatial patterning in CVD;
- Major overhaul of prototype is complete;
- Extensive use of simulation tools for reactor design and interpretation of experimental data