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

<table>
<thead>
<tr>
<th>Authors</th>
<th>Design innovation</th>
<th>Material system</th>
</tr>
</thead>
<tbody>
<tr>
<td>Moslehi, Davis, Matthews (1995)</td>
<td>3 annular zone showerhead</td>
<td>W CVD</td>
</tr>
<tr>
<td>Van der Stricht, Moerman, Demeester, Crawley, Thruch (1997)</td>
<td>Separate TMG, NH3 injection to reduce gas phase reactions</td>
<td>GaN MOCVD</td>
</tr>
<tr>
<td>Theodoropoulos, Mountziaris, Moffat, Han, Shadid, Thrush (2000)</td>
<td>Annual ring showerhead with alternating TMG, NH3 inlet rings</td>
<td>GaN MOCVD</td>
</tr>
</tbody>
</table>

**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:
H₂ reduction of WF₆

- Water temp: 673 K
- Deposition time: 20 min
- Flow: 60 scm/segment

Segment 1: \( x_{H₂} = 0 \), \( x_{WF₆} = 1 \)
Segment 2: \( x_{H₂} = 0.8 \), \( x_{WF₆} = 0.2 \)
Segment 3: \( x_{H₂} = 1 \), \( x_{WF₆} = 0 \)

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

ULVAC vacuum chamber modified for 3-segment prototype
Prototype construction

- Linear motion device
- Gas inlet
- Exhaust port
- One hexagonal segment
- ULVAC CVD chamber
- 4" substrate heater
Prototype construction

Top View:
- CF 8in half nipple internal diam.
- Linear motion device mounted on CF 1.3 flange
- 4" wafer

Bottom View:
- CF Reducing flange from 8" to 2.75"
- Quick disconnect fitting with 1/4" OD gas line
- Outer circle: Seal nut OD
- Medium circle: Weldable body OD
- Inner circle: .25 in gas line
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

<table>
<thead>
<tr>
<th>Seg</th>
<th>Gas Composition</th>
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<tbody>
<tr>
<td>1</td>
<td>50 sccm Ar</td>
</tr>
<tr>
<td>2</td>
<td>50 sccm WF&lt;sub&gt;6&lt;/sub&gt;</td>
</tr>
<tr>
<td>3</td>
<td>50 sccm H&lt;sub&gt;2&lt;/sub&gt;</td>
</tr>
<tr>
<td></td>
<td>0.5 torr</td>
</tr>
<tr>
<td></td>
<td>300-350 C</td>
</tr>
</tbody>
</table>

**Question:** Why does W deposition occur in segments 1 (Ar) and 3 (H<sub>2</sub>)?
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

1. Represent data in XML
2. Java parser methods called from MATLAB applications
4-point probe data analysis

**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 thickness map**
W deposition profiles

Deposition Rate

Dist from WF₆ Seg

Gap size

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Segment transport model

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

\[
\nabla x_i = \sum_{j=1, j \neq i}^{N_i} \frac{1}{CD_{ij}} (x_i \overline{N}_j \nabla x_j \overline{N}_i) \quad \overline{N}_i = N_i + \frac{D_i}{M_i} \nabla \ln T
\]

- 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

\[
\frac{\partial T}{\partial t} = \nabla^2 T - v_x \frac{\partial T}{\partial x} + R_c(T)
\]

\[
T(x, y, t) = \sum_{i=1}^{M} \sum_{j=1}^{N} a_{i,j}(t) \phi_i(x) \psi_j(y)
\]

F.val : \{\phi, \psi\}
F.dir : [1, 2]
F.wt : \{w_x, w_y\}

Overloaded operators and functions

\[
T = a \ast F
\]

\[
\dot{a} = wip(DDX \ast T + DDY \ast T - v_x \ast DX \ast T + R_c, F)
\]

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

**Ar**

**WF$_6$**

**H$_2$**

50 sccm / segment

5 sccm / segment
Deposition pattern control

Increasing across-wafer diffusion
Effect of gap size on film thickness

Intersegment diffusion contribution

Back diffusion contribution

Gap size

Seg 1 (Ar)

Mean deposite, mm/min

Simulation

Data

Seg 3 (H₂)

Mean deposite, mm/min

Simulation

Data

Back diffusion contribution

Ar

H₂
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