A New Approach to Spatially Controllable CVD

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Conventional CVD designs

Chemical Vapor Deposition (CVD) reactors for microelectronics manufacturing

- Precursor chemical species are fed to a reaction chamber and
- React on the heated wafer surface to deposit a thin film of the desired material
Limits of conventional CVD designs

Across wafer nonuniformities in
  • Film thickness
  • Composition
  • Microstructure

Can be difficult to solve because of
  • Inflexible, fixed designs
  • Few control inputs
  • Limited wafer access and few sensors

Result
  • Process/product tradeoff
  • New reactor design for each application
Background: GaN reactor redesign project

UMd/Northrop Grumman collaboration on GaN epitaxy simulator development

Motivation
Poor across-wafer and wafer-to-wafer film nonuniformity

Approach
Characterization of the GaN process to determine critical chemical and transport processes are critical

Gas-phase transport modeling to evaluate reactor design alternatives and interpret sensor signals

Model-based process optimization and re-design
Iterative simulation-based re-design

CVD process operations leading to spatially non-uniform film growth

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

Simulation-based assessment of design and operation alternatives
Evolution of uniformity improvement

- **Process characterization**
  - Thermal modeling
  - Showerhead fluid mechanics
  - Reactor fluid mechanics
  - Reaction kinetics

- **Hole Pattern**: E213-40, A-75, E172, F203, F243
- **Conditions**: G102, G147, G165/96, G226
- **Non-uniformity**: 21%, 22%, 24%, 7.4%, 8% / 6% (rot)

- **GaN Thickness**
  - Winter 2001/02
  - Spring 2002
  - Summer 2002
  - Fall 2002

- **Al Conc**
**Observation:** GaN film spatial uniformity is governed by Ga-species flux at wafer surface and was improved through iterative showerhead redesign.

**Motivation:** develop a reactor design that allows spatial control of gas composition across the wafer surface without physical modifications.

<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>

**Designs above exhaust in “conventional” ways**
Previous efforts at gas composition control

These designs are subject to considerable inter-segment convective transport

Moslehi, Matthews (1995)
Recirculating showerhead design

- Reverse-flow reduces inter-segment interaction
- Concentration profile can be controlled using gap size
- Gas sampling capabilities
Prototype I construction

Three segments and W CVD for proof of concept and engineering data

- Linear motion device
- Feed Gas
- Exhaust gas
- Hexagonal showerhead segment
- Substrate heater
- 100 mm wafer
- Ulvac CVD chamber
- Feed tube
- Hexagonal segment
- Gas sampling tube

Spatially Controllable CVD || 2004 ACC, Boston MA  R. A. Adomaitis, Chem Eng & ISR  7/1/04  10
Gas species transport in the prototype

Back diffusion from common exhaust volume to segments

Gap Region inter-segment interaction affects gas concentration in each segment
Segment transport model

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

\[ \nabla x_i = \sum_{j=1, j\neq i}^{N} \frac{1}{CD_{ij}} \left( x_i \bar{N}_j - x_j \bar{N}_i \right) \]

\[ \bar{N}_i = N_i + \frac{D_i^T}{M_i} \nabla \ln T \]

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

- Create segment model objects for each segment - modularity;

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

- Download operating conditions from data archive website to define modeling objects.
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
Initial experimental testing

Experimental Conditions for W deposition

1. Process pressure = 0.5 torr
2. Wafer temperature = 350 °C
3. Deposition time = 10 min
4. Z = 50 mm (fixed)
5. d = 1, 2, 3 mm
4-point probe data analysis

**Observations**

1. Metrology data confirms existence of W films in Ar and H₂ segments
2. Negative thickness gradient with respect to distance from WF₆ segment
3. Thickness in Ar and H₂ segments grows with gap
Effect of gap size on film thickness

- Intersegment diffusion contribution
- Back diffusion contribution

**Seg 1 (Ar)**

- Ar

**Seg 3 (H₂)**

- H₂

**Gap size**

Mean dep rate, mm/min

Simulation 
Data
Prototype I limitations

While prototype I demonstrated (late 2002) the proof of reverse-flow design:

- Gas sampling not implemented in 1st prototype
- Prototype was subject to various mechanical difficulties, including shifting segments, leaks, etc.
- Primitive gas flow control system to the segments
- System could not be operated where $H_2$ reduction of WF$_6$ is well-understood
1. New clean reactor chamber reduces undesirable reactions (1.0E-8 torr)

2. Extendible reaction chamber (8 inch 6-way cross CF) allows convenient modification of reactor structure.
Prototype II, continued

- Complete reconstruction of 3-zone prototype to improve reliability and achieve true programmability;

3 MFCs/segment
Programmable Reactor goals

• 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
Representative experimental results

Heater T: 400 °C  Chamber P: 1 torr  Gap: 1mm

Intentional seg-to-seg NONuniformity using different recipes in each segment

<table>
<thead>
<tr>
<th></th>
<th>Seg 1.</th>
<th>Seg 2.</th>
<th>Seg 3.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar</td>
<td>0</td>
<td>60</td>
<td>30     [sccm]</td>
</tr>
<tr>
<td>WF6</td>
<td>12</td>
<td>0</td>
<td>6      [sccm]</td>
</tr>
<tr>
<td>H2</td>
<td>48</td>
<td>0</td>
<td>24     [sccm]</td>
</tr>
<tr>
<td>Total</td>
<td>60</td>
<td>60</td>
<td>60     [sccm]</td>
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Representative experimental results

Heater T: 400 °C  Chamber P: 1 torr  Gap: 1mm

Intentional seg-to-seg uniformity (at prev seg 3 conditions)

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[Diagram showing spatial distribution of conditions]
Simulator deposition thickness predictions

Simulator predicts film growth rates much more accurately in new prototype with no adjustable parameters

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<th>Thickness [nm]</th>
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<tr>
<td>1</td>
<td>384</td>
</tr>
<tr>
<td>2</td>
<td>53</td>
</tr>
<tr>
<td>3</td>
<td>250</td>
</tr>
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</table>

Segment 1, 2, 3
Conclusions

- This presentation focused on the design and testing of a new CVD reactor design that allows 2D sensing and control of gas composition across the wafer surface.
- Two, 3 zone prototypes were constructed; initial testing demonstrated the feasibility of spatial patterning in CVD and a step towards programmable control of uniformity characteristics.

Current process control research includes:

- Optimization of model-based programmed nonuniformity for combinatorial studies.
- Real-time distributed end-point control using spatially resolved RGA.
- Run-to-run and real-time compensation for wafer temperature variations due to gas composition differences.
Wafer temperature/RGA characterization

Segment 1

Segment 2

Silicon Wafer

Area covered by segment

0.48 inch

2.0 inch

Segment 3

Ar
60 sccm

N₂
60 sccm

Ar
60 sccm

Heater setpoint 400°C

Gap 32 1 32 1

Signal [AMP]