Integrated Dynamic Simulation for Process Optimization and Control

G. Brian Lu, Laura L. Tedder, Monalisa Bora, and Gary W. Rubloff

NSF Engineering Research Center for Advanced Electronic Materials Process
North Carolina State University, Raleigh, NC 27695-7920

Outline:

• Motivation
  – Process/Equipment Analysis, Design, and Control
• Simulator Structure
  – Dynamic and Physical Approach
  – PolySi RTCVD Simulator Structure
  – Dynamic Characteristics
• Simulator Validation
  – Sensor Signals, Reaction Kinetics
  – Film Deposition
• Applications in Process Optimization for Manufacturing and the Environment
  – Process Cycle Time
  – Materials Utilization Efficiency
  – Other Manufacturing Figures of Merit
• Applications in Manufacturing Education and Training
• Conclusions

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Motivation:

• Both single-wafer and batch semiconductor processes are discrete, fairly short steps

• Transient / dynamic characteristics of process influence properties and reproducibility of product
  – Finite times needed to establish or change process conditions (e.g., start and finish)
  – Variations during nominally steady-state process conditions
  – Transitions between different chemical reaction regimes

• Dynamics may be a crucial factor in designing efficient processes, equipment, sensor, and control systems
Dynamic Simulators for Sensor-Based Process Control

Dynamic simulation to capture time-dependent behavior
Simulators ==> virtual sensor data
Comparison of real and virtual sensor data ==> control
Dynamic Simulation Applications

• Process/equipment design and performance analysis
  – Sensor signal simulation
  – Fault simulation and classification
  – New process recipe
  – New equipment configuration

• Process extension to new parameter regimes
  – Flexible manufacturing

• Manufacturing optimization
  – Process cycle time

• Environmental optimization
  – Materials utilization efficiency
Our Approach to Dynamic Simulation

• Use physically-based models wherever possible
  – Radiative heat transfer
  – Mass balance
  – Boundary layer transport
  – Surface adsorption/reaction/desorption kinetics
  – Growth rate, film thickness

• Use other models elsewhere to complete the system-level description
  – Reduced-order models to represent high complexity (e.g., reactor fluid dynamics, heat transfer)
  – Empirical/statistical models where physics/chemistry poorly known (e.g., plasma process)

• Time-dependent behavior of the equipment and process
  – Real-time based functions for all input and output parameters

• Integration of simulators for equipment, materials/process, sensor, and control system
  – Linked equipment/process/sensor/control simulators through global parameter variables
  – Control system implementation (sequential event driver)
Schematics of Polysilicon RT-CVD Reactor

Gas Handling
Gas cylinder

MFC

heating lamps

SiH₄ → Si + 2H₂

RTP Reactor and Pumps
RTP reactor
RTP pumps

1st stage 2nd stage
pumps
pumps

metering valve

1.0 mm sampling aperture

Mass Spec Sampling
QMS
Windows-based RTCVD Simulator Structure

Compound Block Structure

Second Level Compound Block
Schematics of a VisSim Block-diagram and the Corresponding Mathematical Expressions

\[
N_A^g + N_B^g = \frac{N_A^g}{N_A^g + N_B^g} F \frac{N_A^g}{N_A^g + N_B^g} \int F \frac{N_A^g}{N_A^g + N_B^g} dt + \int F \frac{N_A^g}{N_A^g + N_B^g} dt = N_A^{\text{out}}
\]
Dynamic RTCVD PolySi Simulator

**Process Recipe**
- Valves, MFC’s vs. time, status
- Lamp power vs. time
- Overall process timing, conditions

**Equipment Simulator**

**Sensors and Control**
- Total and partial pressures
- Temperatures
- Valve and MFC status

**Process Simulator**
- PID controllers for temperature and pressure
- Lamp power output control
- Throttle valve positions

**Manufacturing FoM Simulator**
- Cycle time
- Consumables volume
- Energy consumption

**Gas Flow**
- Vacuum chambers
- Mass flow controllers
- Pumps, valves
- Conductances, volumes
- Partial and total pressures
- Pressure control system
- Viscous/fluid flow

**Heat Flow**
- Wafer absorptivity, emissivity
- Wafer thermal mass
- Wafer radiation, conduction
- Wafer temperature
- Temperature control system
- Process-dependent absorptivity, emissivity
- Convective heat loss in fluid flow

**CVD Reaction**
- Gas phase transport
- Boundary layer transport
- Surface-condition-dependent reaction rates - surface kinetics

**Wafer State**
- Deposition rate
- Film thickness
- Thickness control system
- Product properties - uniformity, conformality, material quality, topography, reliability

**Manufacturing Process Efficiency**
- Gaseous emissions
- Reactant utilization
- Power consumption
- Solid waste
Examples of Dynamic Elements

• **Time and history dependent film deposition:**
  – Temperature and partial pressures vary continuously through process
  – Surface reaction and deposition rates vary continuously through process
  – Film thickness depends on detailed process history

• **Process-dependent absorptivity/emissivity and temperature control:**
  – Film thickness changes during deposition
  – Absorptivity/emissivity changes with film thickness
  – Temperature variation is compensated by PID control of lamp power output

• **PID pressure control**
  – PID throttle valve controller stabilizes initial reactor pressure
  – Surface reaction induced pressure change is compensated by PID control of throttle valve position.
Go to “landscape” file for this figure.
Direct Output from the Simulator

• Process time-profile:
  – Partial and total pressures in reactor
  – Wafer temperature and optical properties
  – Reaction rates
  – Deposition rate

• Equipment time-profile:
  – Valves and MFCs
  – Lamp power
  – Control system
  – Sensor signals

• Manufacturing Figures of Merit
  – Film thickness (and quality)
  – Process cycle time and throughput
  – Materials consumption
  – Power consumption

• Environmental Figures of Merit
  – Gas by-product formation
  – Partial pressures in down-stream gas
  – Materials utilization efficiency
  – Process mass balance
Comparison of PolySi RTCVD Film Thickness Between Experimental and Simulation

- Simulator captures dynamic physics and chemistry well to first order
- Some systematic subtleties not yet represented
## Process Optimization for Environmentally Conscious Manufacturing

- To identify where significant gains are possible
- To minimize experiments needed for optimal process design

### Manufacturing Figures of Merit
- Film thickness (and quality)
- Process cycle time and throughput
- Materials consumption
- Power consumption

### Environmental Figures of Merit
- Materials utilization efficiency
- Power consumption
- Partial pressures in down-stream gas
- Process mass balance
Dynamic Simulation for Environmental and Manufacturing Optimization

RTCVD PolySi: **timing and temperature dependence**, 300 sccm

- Higher temperature and earlier wafer heating benefit BOTH manufacturing and environment:
  - higher SiH$_4$ utilization
  - shorter process cycle time
- Dynamic simulation permits quantitative prediction for complex behavior
Dynamic Simulation for Environmental and Manufacturing Optimization

**RTCVD PolySi: timing and flow dependence**

- **SiH₄ Utilization (%)**
  - 100 sccm
  - 200 sccm
  - 300 sccm
  - 450 sccm
  - 600 sccm
  - 1000 sccm

- **Process Cycle Time (sec)**
  - 100 sccm
  - 200 sccm
  - 300 sccm
  - 450 sccm
  - 600 sccm
  - 1000 sccm

- **Pressure (torr) at which heating begins**
  - Start gas flow and heating simultaneously
  - Start heating after gas flow established

- **Lower flow rate and earlier wafer heating:**
  - Higher SiH₄ utilization (reduced consumables cost, environmental benefit)
  - Somewhat higher process cycle time

- **Dynamic simulation permits quantitative prediction for complex behavior**
• Time-dependent physical and chemical behavior determines manufacturing figures-of-merit (FoM’s)
• Multiple manufacturing FoM’s result from equipment, process, control choices and parameters
Dynamic Simulation Applications

• **Equipment design and performance**
  – 3-stage CIS mass spec vacuum system dynamics

• **Process recipe design**
  – Interpolation and extrapolation for multi-parameter process models

• **Sensor signal simulation**
  – Linked equipment/process/sensor simulators
  – Virtual sensor signals to compare with actual signals

• **Manufacturing optimization**
  – Process cycle time, consumables cost

• **Environmental optimization**
  – Reactant utilization efficiency

• **Manufacturing education and training**
  – Modules providing real-time, interactive operator training

• **Design for contamination control**
  – Gas impurity variation with use from liquid source

• **Control systems behavior**
  – PID controls for temperature and pressure

• **Fault simulation**
  – Equipment/process/sensor failure and consequences

• **Dynamic Simulator based equipment/process control**
Simulator Module and Integration for Manufacturing Training and Education

- Dynamic simulator integrated with HELP files to form stand-alone simulator module
- Simulator modules incorporated into manufacturing education and training courses

Dynamic Simulator: MOCVD SYSTEM

Module HELP file

Dynamic Simulator HELP file

Dynamic Simulation Exercise

Course lectures
Conclusions

• Crucial issues for semiconductor manufacturing demand understanding and analysis of complex, multi-variable behavior as a function of time

• Commercial software provides a powerful, versatile vehicle for dynamic simulation

• Dynamic behavior of equipment, process, sensor and control systems are replicated in real-time with physically-based models

• Numerous important applications to manufacturing exist
  – Equipment design and performance
  – Process recipe design
  – Sensor signal simulation
  – Control systems behavior
  – Manufacturing optimization
  – Environmental optimization
  – Manufacturing education and training
  – Fault simulation
  – Design for contamination control