Integrated ESH Assessment: 
Cu CVD Unit Process

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Scope and Strategy

Multilevel modeling & simulation incorporating dynamics & stochastics

Aggregate ESH impact metrics to upper levels

Global

Factory or site

Incorporate capability in models for dynamics & stochastics

Product mix, market dynamics

WIP fluctuations

Subfactory or process-group

ESH infrastructure

Factory, subfactory, & tool logistics

ESH infrastructure loads & control systems

Subfactory

Process & tool

Process recipes at tool level

Fundamental science

Reaction kinetics

Primary research areas of the Center

Optimize ESH impact metrics at multiple levels

Cu CVD example

Incorporate capability in models for dynamics & stochastics
### Integrated ESH Assessment

**Optimize ESH within performance and cost requirements of the industry**

- ESH impact metrics exist within a larger context of product performance and manufacturing metrics.

<table>
<thead>
<tr>
<th>Category</th>
<th>Metrics</th>
<th>Priority/Requirements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Technology Performance</td>
<td>Speed, power, density, yield, reliability</td>
<td>Non-negotiable requirement #1 priority “Hard” constraint</td>
</tr>
<tr>
<td>Manufacturing Productivity</td>
<td>Cost-of-ownership, throughput, cycle time, overall equipment efficiency</td>
<td>Primary productivity optimization #2 priority</td>
</tr>
<tr>
<td>ESH Impact</td>
<td>Materials usage &amp; exposure, emissions &amp; waste, water, energy</td>
<td>Highly desirable, but #3 priority</td>
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</table>

- **Seek common methodology for assessing and optimizing performance, manufacturing, and ESH metrics**
  - *Respect product performance requirements*
  - *Develop ESH improvements which minimize cost impact and may improve manufacturing productivity (“dual-use”)*
  - *Stimulate innovation through efforts to co-optimize manufacturing and ESH metrics*
Dynamic Simulation

Multi-level Hierarchical Structure

User-friendly Pop-Up Panels for Real-Time Process & Equipment Parameters Control

Real-Time Monitoring of the DYNAMIC Behavior of Equipment, Process, & Control System through Process Cycle

Real-Time Monitoring of the DYNAMIC Behavior of Manufacturing Efficiency & ESH Assessment Metrics

Both Digital & Graphical Representation of Data

Real-Time Monitoring of the Arrhenius & "Arrhenius-Pressure" Curves generation
Dynamic Simulator for Cu CVD Process

- Dynamic Simulation can realistically represent complex systems, including:
  - equipment
  - process
  - sensors
  - control
- Results validated against experiment:
  - timing / dynamics
  - subtle systematics
- Numerous applications:
  - systems analysis
  - optimization
  - sensor-in-tool models
  - control system design
  - training / learning
Components of the Dynamic Simulator for Cu CVD Process

- **PROCESS RECIPE**
  - Set Points: Total Press, Flow Rates of Precursor & Carrier Gas as a func of Process Timing
  - Set Points: Process Temp
  - Valves, MFC's status as a func of Time

- **EQUIPMENT SIMULATOR**
  - Vacuum Chambers, Pumps, Valves, MFC's, Direct Liquid Injection System
  - Process Pumping Stack:
    - Roots Pump, Root-Blow Pump, Scrubber
  - Conductances, Volumes, Press Control System
  - Thruputs, Residence Time, Concentrations of Reactant, Carrier Gas, & Gaseous By-Products
    - TOTAL & PARTIAL PRESSURES
  - Substrate Heater Controller:
    - Heater & Wafer Absorptivities, Emissivities, Thermal Conductivities, Thermal Masses, Conduction, Radiation, Process-dependent Absorptivity & Emissivity, Heat Capacities,
    - Temp Control System

- **PROCESS SIMULATOR**
  - CVD Reaction:
    - Gas Phase Transport
      - transport rate coeff ➔ Rate of Transport
    - Surface Reaction Kinetics
      - surface rxn rate constant & coeff
      - activation energy
      - ➔ Rate of Surface Rxn
    - EFFECTIVE RATE OF RXN

- MANUFACTURING & ESH SIMULATOR

**REAL-TIME FILM THICKNESS CONTROL**

- Deposition Rate, Film Thickness – vs. Time
- Mass Balance, Reactant Utilization, Cycle Time, Power required, Energy expended (per unit thickness)
Components of the Dynamic Simulator for Cu CVD Process

- Deposition Rate as a func of Time
- Film Thickness as a func of Time
- Product Properties: Resistivity, Uniformity, Conformality, Topography, Reliability, etc.

• CONTROL SYSTEM
  - Real-Time Film Thickness Process Control
    - When Film Thickness reaches the Control Thickness, Process is terminated
      - Press SetPt, Reactant & Carrier Gas
      - Flow set to 0
      - Throttle Valve set to Full-Open
  - Simulator Control
    - At the end of the process, when Chamber Press reaches 0,
    - Terminates the updating process for all Dynamic Outputs including Manufacturing & ESH Metrics

• MANUFACTURING & ESH SIMULATOR
  - Manufacturing Process Efficiency:
    - Mass Balance (Consumables, By-Products Generation) ➔ Reactant Utilization
    - Cycle Time
    - Power required
    - Energy expended (per unit thickness)
  - ESH Assessment:
    - Gaseous By-Products Emission
    - Reactant Utilization
    - Energy expended (per unit thickness)
Blanket Cu CVD Process

\[ 2 \text{Cu}^{I}(\text{hfac})(\text{tmvs}) \rightarrow \text{Cu}^0 + \text{Cu}^{II}(\text{hfac})_2 + 2(\text{tmvs}) \]

Available as Schumacher CupraSelect™ Liquid at R.T.

\text{tmvs} = \text{trimethylvinylsilane C}_{5}\text{H}_{12}\text{Si}
\text{hfac} = \text{hexafluoroacetylacetonate dihydrate C}_{3}\text{H}_{6}\text{F}_{6}\text{O}_{2}

Delivered to the showerhead using DLI system.

**RANGE OF PROCESS CONDITIONS FOR SIMULATION EXPERIMENTS**

**PROCESS CONDITIONS FOR SIMULATION**

- Substrate Temp 150 - 250°C (180 - 200°C)
- Vaporizer, Gas Lines and Chamber at 60-65°C.
- Ar/He CarrierGas Flow 50 – 500 sccm (100 sccm)
  
  - **CupraSelect™ Liquid Flow**
    - 0.1 – 0.25 cc/min (for seed 200 - 500 A)
    - up to 2.5 cc/min (for fill 200 - 500 nm)

  - Max Chamber Pressure Defined by DLI Physics
    - In general, < 10 Torr (for seed) & < 4 Torr (for blanket fill)
    - for low CarrierGas Flow Rate (50-100 sccm), and Higher Pressures for higher CarrierGas Flow Rates (upto 500 sccm)

**ARRHENIUS CURVE SIMULATION** – Effective Rate of Rxn composed of Transport-limited & SurfaceRxn-limited Regimes

**“ARRHENIUS PRESS CURVE” SIMULATION** – Pressure-dependence of Growth Rate at fixed Temp & Flow Rates

**simulation model incorporates details of known process chemistry**

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Dynamics of Manufacturing Metrics

**CYCLE TIME**

*Composed of Raw Process Time & Overhead Time*

**Raw Process Time:** Time during which actual film growth is occurring on the wafer

- time for initial chamber filling to press set-pt
- process time during which total & partial pressures have reached more or less steady-state
- time for process gases pump-out at the end of the deposition process

**Overhead Time:** All other time during which there is no deposition on the wafer taking place

- initial “wafer-temp-stabilization time” inside the chamber before process gases are introduced
- wafer loading & unloading Time

**Desired process conditions for Short Cycle Time in general:**

- High Press, High Temp, High Flow Rate ➔ High Growth Rate ➔ SHORT CYCLE TIME

*In general, w/ all other variables fixed, HIGH REACTANT UTILIZATION means SHORT CYCLE TIME (but, not always)*
Dynamics of Manufacturing & ESH Metrics

• **REACTANT UTILIZATION**
  - *Precursor Mass Balance:*
    - # of moles of Precursor IN
    - # of moles of Precursor OUT
    - # of moles of Precursor RXTED to produce product film on the wafer
    - Precursor utilization = RXTED / IN (%)
  - Desired process conditions for High Reactant Utilization in general:
    - High Total Press, High Reactant Partial Press, High Temp, Low Flow Rate
    - Increased Residence Time, High Growth Rate
    - HIGH REACTANT UTILIZATION

• **POWER & ENERGY**
  - *Sources of Energy Use:*
    - Substrate Heater, Process Pumps, Process Chamber, Vaporizer & Gas Lines Heating, DLI System Pumps, Pre-Heated Precursor, Process & Equipment Control Units, PC’s, etc.
  - *Substrate Heater:*
    - Heater kept at high temp at all times
    - Significant portion of Energy lost during Overhead Times
    - Radiative Heat Loss \( \sim (T_2)^4 \)
    - Conductive Heat Loss \( \sim (T_2-T_1) \)
Process Cycle Time

- Manufacturing

PRESS: 5, 10, 20, 30, 40 TORR
CONST FLOW RATES 1 CCM / 200 SCCM

FLOW RATES (CCM/SCCM): 0.5/100, 1.0/200, 1.5/300, 2.0/400, 2.5/500
FIXED FLOW RATIO: 1CCM/200SCCM
CONST PRESS: 10 TORR

Cycle Time (min) vs. Temp (°C) for different pressures and flow rates.
Reactant Utilization

PRESS: 5, 10, 20, 30, 40 TORR
CONST FLOW RATES 1 CCM / 200 SCCM

FLOW RATES (CCM/SCCM): 0.5/100, 1.0/200, 1.5/300, 2.0/400, 2.5/500
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CONST PRESS: 10 TORR
Unit Process Optimization for Cycle Time & Reactant Utilization

- High Press, High Temp: Win-Win Situation for Cycle Time & Utilization
- In the case of Flow Rate: Trade-off between Cycle Time & Utilization exists

FLOW RATES: 0.5/100, 1.0/200, 1.5/300, 2.0/400, 2.5/500
FIXED FLOW RATIO: 1 CCM/200 SCCM
TEMP RANGE: 150 – 250°C
CONST PRESS: 10 TORR

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TEMP RANGE: 150 – 250°C
CONST FLOW RATES 1 CCM/200 SCCM
Power & Energy

**Temp-dependence of power input**

Radiation (~$T^4$) and conduction (~$\Delta T$) are both important heat transfer channels in the process temperature regime for Cu CVD. Maintaining higher temperature incurs higher power input. ➔ expect to prefer lower temperature to save energy.

**ENERGY OPTIMIZATION**

Temp-dependence of RxnRate is strong (exponential)

➔ higher temp causes shorter cycle time
➔ shorter cycle time reduces energy cost

Temperature dependence of energy usage is dominated by cycle time effect, not by power needs for maintaining wafer temperature in the process temperature regime for Cu CVD.
Cu CVD Unit Process Optimization for Manufacturing & Environment

- **MANUFACTURING METRICS**
  - PROCESS CYCLE TIME
  - ENERGY EXPENDED PER UNIT THICKNESS

- **ESH METRICS**
  - REACTANT UTILIZATION EFFICIENCY
  - ENERGY EXPENDED PER UNIT THICKNESS

- **PROCESS PARAMETERS**
  - TEMPERATURE
  - PRESSURE
  - FLOW RATE

- **CO-OPTIMIZATION OF MANUFACTURING & ESH METRICS**
  - Energy (~Cycle Time, Throughput)
  - Mass balance = reactant utilization (no emissions/waste yet)

- **CAN OPTIMIZE ESH METRICS WITHIN THE RANGE OF OPTIMAL MANUFACTURING PROCESS CONDITIONS**
# Future Plans

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<th>Unit process</th>
<th>ESH infrastructure</th>
<th>Subfactory or process-group</th>
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<td>UMd</td>
<td>Cu fill: plating vs. CVD</td>
<td></td>
<td>Cu fill technology roadmap</td>
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<tr>
<td></td>
<td>Water recycling (NSF educ suppl)</td>
<td></td>
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</tr>
<tr>
<td>UCB</td>
<td>CMP process</td>
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<td>CMP recycling (AMAT)</td>
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</table>
Subfactory – Cu Fill
Technology Roadmap

- NSF/SRC program in Operational Methods ➔ integrated modeling structures which couple process and operational models
- W plug example: unit process ➔ cluster tool ➔ subfactory (process-group)

Models and Simulators
- Continuous & discrete-event
- Static and dynamic
- Empirical and physics-based
Vision & Project Objectives

• **DFE methodology for assessing & optimizing ESH impact metrics** from the science plane to the factory level
  – *Create models to assess ESH metrics at multiple levels*
    o Unit process, equipment & recipe, ESH infrastructure, subfactory
  – *Compare ESH metrics for*
    o Conventional processes, with and without ESH infrastructure enhancements
    o Alternative processes
    o Emphasize integrated assessment at higher levels and sensitivity analysis (systems picture)

• **Systems engineering** approach to achieve ESH benefits within the larger context of product performance and manufacturing metrics
  – *Develop models which reveal metrics for performance & manufacturing as well as ESH*
  – *Co-optimize where possible; understand and prioritize tradeoffs elsewhere*

• **Systemic implementation of DFE** across the Center’s research portfolio
  – *Apply DFE methodologies across portfolio of CEBSM projects, in collaboration with or driven by project participants*
  – *Reinforce learning and practice in research projects and educational programs*
Conclusion

• Cu CVD unit process model established and used to assess ESH and manufacturing metrics
  – Mass balance limited to reactant utilization (not including emissions/waste)
  – Energy balance reveals non-intuitive results from competing factors

• Modeling approach provides platform for optimization and tradeoff analysis for multiple metrics
  – Additional metrics are important to incorporate
  – Film quality, emissions/waste, ...

• Methodology extendible
  – Other unit processes (Cu plating, CMP, ...)
  – Subfactory or process-group
  – ESH infrastructure