Faculty Presentation: CMP

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Current Milestones

- **Nanomechanics of surface polishing**
  - Analysis of surface interactions during nanoscale polishing - multi-scale mechanistic/stochastic approach

- **CMP Electrochemical Effects**
  - Mechanism for coupling of chemical and mechanical phenomena in CMP
  - Develop chemical models to characterize the material removal due to chemical/electrochemical effects and integrate into comprehensive CMP model
  - Basic material removal model development: Mechanism for discrete material removal at pad/wafer contact including influence of pad topography

- **Comprehensive model development**
  - Identify key influences of chemical and mechanical activity with the assistance of the fundamental studies

- **Effects of slurry chemistry on agglomeration and surface hardness**
  - Continue to develop basic understanding of agglomeration/dispersion effects on CMP - study rate of agglomeration as a function of chemistry.
Outline

- Mechanics of Nanoscale Polishing (Komvopoulos)
- In-situ process monitoring for CMP (Dornfeld)
- Integrated CMP models
  - Impact of colloid behavior on MRR with “additive” model that considers both mechanical and chemical factors
  - Impact of asperity-wafer and abrasive-wafer interaction frequency in “synergistic” model that treats CMP as wear-enhanced corrosion process (new approach to modeling)
Chemical Mechanical Planarization - Faculty Team

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Mechanical Phenomena

Interfacial and Colloid Phenomena

Chemical Phenomena
Chemical Mechanical Planarization - Student Team

Mechanical Phenomena

Chemical Phenomena

Interfacial and Colloid Phenomena

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Mechanics of Nanoscale Polishing (Lapping) – Implications in Magnetic Recording Heads

- Increasing demands for extremely high-density recording have yielded very tight tolerance requirements for the head-disk interface, hence leading to the requirement of ultra-smooth (rms < 0.2 nm) recording head surfaces.

- Optimization of the lapping/polishing process to achieve extremely high-density recording– with direct implications to all technologies relying on surface smoothness and flatness.

- Development of mechanics models for particle embedment and material removal during lapping/polishing process.
Part A – Nanoscratching Experiments

- **Parameters:**
  - Load: 4 mN
  - Velocity: 0.2 µm/s
  - Scratching distance: 6 µm
  - Conical diamond tip of radius =1 µm

- **Friction Coefficient:** \( f = \frac{F_{\text{lateral}}}{L} \)

**63%Al_2O_3 & 37%TiC:** \( f = 0.1565 \)

**64%Al_2O_3 & 36%TiC:** \( f = 0.1228 \)
Part A – Nanoscratching Experiments (cont’d)

- Wear Coefficient:

\[ k = \frac{HV}{LS} = \frac{HA}{L} \]

63%Al₂O₃ & 37%TiC
\[ A = 2505 \text{ nm}^2 \]
\[ k = 1.25 \times 10^{-2} \]

64%Al₂O₃ & 36%TiC
\[ A = 1789 \text{ nm}^2 \]
\[ k = 8.95 \times 10^{-3} \]
Part B – Analytical Work

- **Lapping process**
- **Input:**
  - Load
  - Particle sizes
  - Velocity
  - Roughness of sample surface and lapping plate
- **Output:** surface roughness and material removal rate

**Computational Scheme:**

1. Calculate gap distance:
   \[ h = F^{-1}(L, f(z'), f(z''), f(R)) \]
2. Material removal based on wear criterion
3. Calculation of roughness & material removal rate
Single-Asperity Contact Model

single asperity: \( F_s = p_m a_r \cos \theta \)

Total Force: \( L = \sum F_s \)

\[
F = F(h, f(z'), f(z''), f(R))
\]
\[
h = F^{-1}(L, f(z'), f(z''), f(R))
\]

known variables \((a, d, V_{cap}) \Rightarrow \delta / r'\)

\[
\begin{align*}
(1) & \text{ elastic deformation: } \delta / r' < 1.78(E/Y)^{-1} \\
& \frac{p_m}{Y} = \frac{4\sqrt{2}}{3\pi} \left( \frac{E\delta}{Yr'} \right) ; \quad a_r = 0.5 \\
(2) & \text{ elastic–plastic deformation: } 1.78(E/Y)^{-1} \leq \delta / r' \leq [1 + 0.037(E/Y)]^{-1} \\
& \frac{p_m}{Y} = 0.839 + \ln \left( \frac{E}{Y} \right)^{0.656} \left( \frac{\delta}{r'} \right)^{0.651} ; \quad a'_r = 2.193 - \ln \left( \frac{E}{Y} \right)^{0.394} \left( \frac{\delta}{r'} \right)^{0.419} \\
(3) & \text{ plastic deformation: } \delta / r' > [1 + 0.037(E/Y)]^{-1} \\
& p_m = H ; \quad a_r = a'
\end{align*}
\]
3D Probabilistic Lapping Model

- **Parameters:**
  - Normal Load
  - Topography of workpiece surface (fractal surface description)
  - Particle distribution (size, height, and spacing)
  - Topography of lapping plate

- **Wear Criterion**
  - Elastic deformation: no wear
  - Elastic-plastic deformation: plowing without wear
  - Plastic deformation: cutting

- **Diamond particles on tin lapping plate:**
  - Stable particles: \( L \leq L_{\text{max}} = H_{\text{tin}} \times \pi R^2 \)
  - Sinking particles: \( L > L_{\text{max}} \)
Reconstruction of workpiece surface

- **Fractal surface**: continuous, nondifferentiable, self-affine

\[
z(x, y) = L \left( \frac{G}{L} \right)^{(D-2)} \left( \frac{\ln \gamma}{M} \right)^{1/2} \sum_{m=1}^{M} \sum_{n=0}^{n_{\text{max}}} \gamma^{(D-3)n} \left\{ \cos \phi_{m,n} - \cos \left[ \frac{2\pi \gamma^n (x^2 + y^2)^{1/2}}{L} \cos \left( \tan^{-1} \left( \frac{y}{x} \right) - \frac{\pi m}{M} \right) + \phi_{m,n} \right] \right\}
\]

- **Workpiece surface topography**:

Before lapping
(RMS = 4 nm)

After lapping
(RMS = 3 nm)
Simulation Results

- **Effect of applied pressure**

![Graph](image)

- **Conclusion:**
  - Final roughness of workpiece surface and material removal rate increase with applied pressure.
Simulation Results (cont’d)

- **Effect of lapping plate surface roughness**

  ![Graph 1](image1.png)  ![Graph 2](image2.png)

  - **Conclusion:**
    - Increasing roughness of lapping plate surface would increase the final roughness of workpiece surface but have little effect on material removal rate.
In-situ Process Monitoring for CMP

Motivation

• The ability to predict the effect of changes in parameters during the CMP process should be expanded
  • The development of robust models for CMP remains challenging
  • In-situ metrology is extremely limited

• In-situ process monitoring requires:
  • Appropriate sensor types and systems
  • Interoperability

2008 Objectives

• Study sensor types suitable for in-situ monitoring, including:
  • Thermal
  • Friction
  • Acoustic emission

• Develop interoperability adapters for:
  • MTConnect
  • IPC CAMX

• Develop monitoring package
Multiple types of sensors and local monitoring needed

<table>
<thead>
<tr>
<th></th>
<th>End Point Detection</th>
<th>Head Zone Pressure</th>
<th>Micro-scratching</th>
<th>Pad Condition/Wear</th>
<th>WIWNU</th>
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<tbody>
<tr>
<td>Acoustic Emission</td>
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</table>
Prior AE Research for CMP

- Endpoint detection
- Micro-scratch detection
- Multi-sensor systems

AE RMS signal for SC112 silica based slurry with fine Al₂O₃ particles (Tang et al. 1998)

AE RMS endpoint detection for STI CMP (left) and Cu damascene CMP (right) (Lee et al. 2006)
Current AE Research

- Verifying and expanding endpoint detection
- Development of deterministic methodology for micro-scratch detection
- Monitoring of in-situ pad conditioning
- Expanding use of AE in multi-sensor monitoring systems

Integration of AE sensor into wafer head of CMP machine (Schematic from Lee et al. 2005)

Current AE integration in wafer carrier head of CMP machine; AE sensor is marked with red box

Back side

Front side
MTConnect Architecture

Courtesy of Armando Fox and William Sorbel
Proposed Scheme for CMP

- G&P Poli 500
  - IR Thermal Sensor
  - Piezoelectric Friction Force Sensor

- National Instruments DAQ Card
  - LabView Monitoring Interface
  - Data: Temperature, Friction Force

- IPC CAMX Environment
  - IPC CAMX Plug-in

- CMP Monitoring Software

- MTConnect Agent
  - LabView Adaptor
High cost of ownership process; need to
• Increase removal rate
• Decrease consumable use
• Increase yield
Need predictable, robust, high yield process

Current Slurry/Process design empirical:
Doesn’t meet new requirements
e.g. CMP of copper on porous low-K dielectrics causes failure:
• need new low down-force CMP process

- Dishing & erosion < 10% interconnect height
  - Some success in predicting & controlling for a fixed process
  - Process optimization absent

Volinsky et al. 2003
Colloidal behavior of abrasive particles in CMP

Objective - Understand effects of slurry chemistry on Cu CMP process
- Colloidal behavior measured by zeta potential and agglomerate size distribution - effects of chemical additives and presence of copper
- Studied effects of slurry chemistry on copper surface hardness and etch rate
- Infer state of the Cu (Cu, CuO, Cu2+, etc.) in slurry and on surface
- Used agglomerate size distribution, nanohardness and etch rates in Luo & Dornfeld model of CMP

Current Effort
Continue to develop basic understanding of agglomeration/ dispersion effects on CMP
- Study rate of agglomeration as a function of chemistry
- Investigate effects of heating(temperature) on agglomeration as a function of chemistry

Modeling
- Develop rate of agglomeration model as a function of chemistry which includes the effects of heating (temperature)
- Incorporate rate of agglomeration and heating effects into Luo and Dornfeld CMP model
- Other Models?
# Nanohardness and Etch Rates

## Etch rates and nanohardness with indentation depth <80nm

<table>
<thead>
<tr>
<th>Aqueous solution with 1mM KNO₃ plus:</th>
<th>pH</th>
<th>Etch rate (±4nm/min)</th>
<th>Hardness for &lt;80nm indentation depth (±0.3GPa)</th>
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</thead>
<tbody>
<tr>
<td>none</td>
<td>2.9</td>
<td>0.7</td>
<td>1.6-4.6</td>
</tr>
<tr>
<td></td>
<td>8.3</td>
<td>0.0</td>
<td>1.8-5.7</td>
</tr>
<tr>
<td></td>
<td>11.7</td>
<td>2.6</td>
<td>2.0-7.3</td>
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<tr>
<td>0.1 M glycine</td>
<td>3.1</td>
<td>1.2</td>
<td>1.0-3.5</td>
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<tr>
<td></td>
<td>8.5</td>
<td>7.6</td>
<td>1.6-5.2</td>
</tr>
<tr>
<td></td>
<td>10.0</td>
<td>0.0</td>
<td>3.5-16</td>
</tr>
<tr>
<td>0.1 M glycine, 0.1 wt% H₂O₂</td>
<td>3.0</td>
<td>45</td>
<td>1.0-4.4</td>
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<td></td>
<td>8.3</td>
<td>33</td>
<td>2.1-5.6</td>
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<td></td>
<td>10.1</td>
<td>14</td>
<td>0.34-4.7</td>
</tr>
<tr>
<td>0.1 M glycine, 2.0 wt% H₂O₂</td>
<td>3.0</td>
<td>38</td>
<td>2.8-8.2</td>
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<tr>
<td></td>
<td>8.3</td>
<td>56</td>
<td>0.1-5.5*</td>
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<tr>
<td></td>
<td>10.0</td>
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<td>2.3-18</td>
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<tr>
<td>Combination w/ glycine</td>
<td>3.0</td>
<td>1.6</td>
<td>1.2-3.3</td>
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<tr>
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<td>8.4</td>
<td>0.0</td>
<td>1.7-5.3</td>
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<tr>
<td></td>
<td>10.8</td>
<td>8.6</td>
<td>2.0-4.0*</td>
</tr>
<tr>
<td>Combination w/ EDTA</td>
<td>2.6</td>
<td>0.0</td>
<td>0.9-11*</td>
</tr>
<tr>
<td></td>
<td>9.0</td>
<td>0.0</td>
<td>2.5-8.0</td>
</tr>
<tr>
<td></td>
<td>10.9</td>
<td>0.0</td>
<td>2.1-13</td>
</tr>
</tbody>
</table>

*Values are different than Cu metal for indentation depths >80nm

## For some cases:
- Solutions with large etch rates (>14 nm/min) have soft (possibly porous) films
- Solutions without etching had harder films
- For most cases the hardness was that of Cu metal at indentation depths >70nm

# Hardness sensitive to chemistry!

(depends on pH, etch rate, and chemical additives)
Overall mass material removal (MRR) rate during CMP:

\[ MRR = \rho_w NV + C_0 \]

where \( \rho_w \) = density of copper surface (g/m\(^3\))
\( N \) = number of active abrasives
\( V \) = average volume removed by a single abrasive (m\(^3\)/min)
\( C_0 \) = removal due to chemical etching (g/min)

*Assume Solid-Solid contact mode

Model used experimental values of:
\( x_{\text{avg}} \) – average abrasive size
\( \sigma \) – standard deviation of abrasive size distribution
\( H_W \) – wafer surface hardness
\( C_0 \) – etch rate
Model Predictions

Experimental and model MRR predictions using 1mM KNO₃, 0.1M glycine and 0.1wt% H₂O₂ solution

- Model predictions do not agree with experiment for all pH values
  - At low pH, meas. Hₗ is too small
  - At pH>8, solution in very chemically active (large etch rates >8nm/min), model is very sensitive to Hₗ
    - Hₗ under quiescent conditions different from Hₗ during CMP
    - Surface film too thin to measure using our technique
Model Sensitivity

- Small changes in $x_{\text{avg}}$ or $\sigma$ can cause large differences in predicted MRR.

For small MRR predictions, the model is insensitive to $H_w$, and for large MRR predictions, the model is very sensitive to $H_w$. 
Agglomerate Size Distribution

Cabot alumina dispersion in 1mM KNO₃ solution with (red) and without (blue) 0.12 mM copper and without chemical additives

pH 2 – presence of copper causes **decrease** in agglomeration
pH 7 – presence of copper causes **increase** in agglomeration
Rate of Agglomeration Results

Solutions with Copper

Agglomerate sizes remain relatively constant at pH 4

Agglomerate sizes increase over time at pH 7.5, with agglomerates becoming too large to measure after ~1 hr

Measurements made by Michael Chan
Conclusions on additive model

Nanohardness and Etch Rates of Copper Surface
• Surface hardness is very sensitive to the chemistry of the solution
• State of copper on surface is generally consistent with potential-pH equilibrium diagrams

Modeling MRR Using Luo and Dornfeld Model
• MRR predictions agree better with experiment for slurries that are not very chemically active (etch rate <10 nm/min)
• Surface hardness measurements performed in this study may not be representative of surface hardness that occurs during a CMP process; predictions may or may not improve using the measured $H_W$

• Effect of pH and Copper on Agglomeration
• Rates of agglomeration are sensitive to slurry pH
• Copper has little effect on agglomeration at low pH, but causes slurries at a pH nearer the IEP or higher to agglomerate more quickly
**Synergistic model for copper CMP, based on wear-enhanced corrosion**

Existing mechanism studies and models inadequate

<table>
<thead>
<tr>
<th>Modeling</th>
<th>Mechanism Studies</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Primarily from mechanical perspective</td>
<td>• Primarily from electrochemical perspective</td>
</tr>
<tr>
<td>• Many fundamental physical parameters not measured</td>
<td>• Intermittent nature of the mechanical phenomena not quantitatively considered</td>
</tr>
<tr>
<td>• Continuum treatment of material behavior</td>
<td>• Time and space averaged behavior measured</td>
</tr>
<tr>
<td>• Assume that the chemical reaction rates are not influenced by the mechanical interactions</td>
<td>– Transient electrochemical behavior not measured</td>
</tr>
</tbody>
</table>

**Objectives:**

- Fundamental quantitative understanding of the physical mechanism
  - synergy between mechanical and electrochemical phenomena
- An integrated modeling approach
Copper CMP: at abrasive scale

Mechanical interaction: frequency and force

Mechanical removal response of passive film

Passive film thickness removed, \( \Delta \), Å

Force on an abrasive, nN

Passive current density \( i(t') \), mA/cm²

Passive film thickness (L) (nm)

Time (t') ms

Force (nN)

Relative motion of pad and wafer

Pad asperity

Force

Copper dissolution

Abrasive

Interaction frequency

Force on an abrasive, nN

Bare copper

Passivation kinetics: passive film growth and oxidation rate decay

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10/29/2008
Mechanical Interaction: Frequency & Force – at pad asperity scale

Pad Properties:
elasticity & hardness (both likely influenced by slurry), roughness, porosity

down-force (~1-5psi)

Relative pad-wafer velocity (~1m/s)

Mechanical parameters for the model:

- Asperity interaction frequency: ~1ms
  - duration of contact: ~10µs

- Real contact pressure: ~100psi

C-RICM image of real contact area [1]


Contact ratio response to pressure for 3 different pads [1]

Pad Muldowney, MRS Symp. Proc. Vol. 816


Real contact area

Size & distribution

200 µm

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CMP at Abrasive Scale using an Environmental AFM

Measure response of passive films to ~10nN abrasive force

Asperity interaction frequency: ~1ms
Cu CMP removal rate: ~10nm/s
≡ 0.1-1Å Cu per asperity stroke!!!
(Cu atomic radius = 1.4Å)

- Using an Environmental AFM: the AFM tip can act like an abrasive particle – to scratch copper in

AFM image of copper in air
Image size: ~1µm x 1µm
Mechanical Properties of Passive Film using an AFM

- Solution: 0.1M NaNO$_3$, pH 3, 0.01M BTA, 0.01 M glycine
- Net number of scratches = 210

Solution:
- Pit size 460nm square
- Pit cross section
- z range = 4.7nm
- Force = 9.3 nN

Removal = \( \frac{Z_{\text{surrounding}} - Z_{\text{scratch-area}}}{\text{area}} \)

Expected passive film removal:
- Threshold force
- Saturation

\[ x = y \text{ range} = 1.2 \mu m \]
Passivation Kinetics: Polarization in passivating and inhibiting (BTA) solutions

copper in pH 12 aqueous solution containing 0.01M glycine:
- passivation due to cupric oxide (CuO)

copper in pH 4 aqueous solution containing 0.01M glycine: with and without BTA – effect of scan rate
- very strong inhibition from BTA
Passivation Kinetics in inhibiting (BTA) solution

- Current decay has a very consistent shape throughout
  Decay rate of 0.5 orders per time decade – precisely (Cottrell behavior). Consistent with transport of BTA to copper surface
- Current decays similarly for ‘cathodic’ potential also (below -0.1V)
- There’s no capacitive charging: $RC = 0.2\text{ms}$ (from EIS)

Current decay in absence of BTA, is entirely due to capacitive charging; proved using:
- Electrochemical Impedance Spectroscopy (EIS)
- Simulations

Current decay after stepping potential from -1.2V to different potentials, copper in pH 4 aqueous solution containing 0.01M glycine and 0.01M BTA
Passivation kinetics in passivating solution: the hydrogen peroxide connection

copper in pH 12 aqueous solution containing 0.01M glycine

Evolution of potentiostatic polarization curves over time: in passivating solution

Chronoamperometry:
• Initial currents higher by about 2 orders than corresponding polarization data
• Current decays by greater than 3 orders over 100s
Tribo-Chemical Model of Copper CMP*

1. Passivation kinetics
   Film growth kinetics

2. Mechanical removal response of passive film
   Force & frequency

3. Abrasive-copper interaction
   Force & frequency

Interval between two abrasive-copper contacts ($\tau$)

Removal Rate (nm/s)

$RR = \frac{M_{Cu}}{\rho n F \tau} \int_{t_0}^{t} i(t_0 + t) dt$

$M_{Cu}$: Atomic mass of copper
$\rho$: density of copper
$n$: # e- transferred
$F$: Faraday's constant

$L(t_0 + \tau) - L(t_0) = \Delta L$  (since $L(t')$ is concave)

Test model using fixed abrasive pad, to provide interactions of known frequency and force

- Blanket copper wafers are polished by fixed abrasive pad using rotary CMP machine.

- Three different rotational speeds of platen and head are chosen to investigate the effect of asperity and wafer interaction frequency:
  - Average interval between consecutive wafer-asperity contact, $\tau$: 2.052 ms (for 50 rpm)
  - Duration of contact: 0.214 ms (for 50 rpm)

- Two solutions are prepared to investigate effect of passivation kinetics on MRR:
  - pH4, 0.01 M glycine, 0.01 M BTA and 1 wt% H2O2 in DI water
  - pH12, 0.01 M glycine and 1 wt% H2O2 in DI water

- Copper film thickness measured using four point probe.
Results: Material Removal Rate

- Material removal rate increases as the rotational speed of the platen and head increases.
- Material removal rate is much higher in pH 12 solution than in pH 4 solution.
Effect of Abrasive-Asperity-Copper Interaction Frequencies

- Frequency of abrasive-wafer interactions much higher than that of asperity-wafer interactions, but duration much less. Can combine passive film removal from multiple abrasive contacts under the same asperity, and by the pad asperity itself, into a single parameter.

- Comparing material removal during $2\tau$ for both cases, material removal for doubled interaction frequency is larger, but not necessarily double because of non-linear copper dissolution kinetics and passive film formation kinetics.
Passivation Kinetics of a pH12 solution

- Copper in this solution forms a protective passive film that is removed by asperities and abrasives during CMP

Current decay of copper in pH12 0.01M glycine, 10^{-4}M CuNO_3

Potentiodynamic polarization curves of copper at pH12, 0.01M glycine, 10^{-4}M CuNO_3 obtained at two different scan rates

*Shantanu Tripathi, PhD thesis, UC Berkeley, 2008
Passivation Kinetics of a pH4 solution

- Copper in this solution does not form a passive film, but the inhibitor BTA forms a protective film on the copper surface. This is removed by abrasion.

Current decay of copper in 0.01M glycine, 10^{-4}M CuNO_3, pH4, 0.01M BTA*

Potentiodynamic polarization curves of copper, 0.01M glycine, 10^{-4}M CuNO_3, at pH4 (0.05M buffer) with and without BTA*

*Shantanu Tripathi, PhD thesis, UC Berkeley, 2008
Conclusion: Integrated tribo-chemical modeling
Future Work

- Simulation of removal rate using the model – Monte Carlo method
- Verification with experiments

Multi-scale Pattern Dependency Modeling

Material Removal Model

$$RR = \frac{M_{cm}}{\rho(t)} \int t dt$$

- Consumables
- Polishing Conditions

Multi-scale CMP optimization

- Change pad hardness (tree level 1)
  Inflexibility: scratch defects, pad supplier

- Change incoming topography (feature level)
  Inflexibility: deposition process limitation

- Dummy fill (chip array level)
  Inflexibility: design restrictions

- Change chemical reactions, abrasive concentration (abrasive level)
  Inflexibility: removal rate requirements

- Within die non-uniformity
  Nitride Thinning in STI

- Asperity contact area ($\mu m$)
  Empirically fit, based on pad flexion (scale=mm)

- Recalculate effective pattern density

- Space Discretization: Data Structure

- Time step evolution

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Future Milestones

- **Nanomechanics of surface polishing**
  - Optimization of nanoscale polishing and implications in CMP

- **Comprehensive model development**
  - Development of strategies for model-based process optimization for use in the “manufacturing pipeline” (e.g., DfM), as with pattern dependency effects.

- **Fundamental mechanical effects**
  - Analysis of pad mechanical behavior, details of pad topography, FEM analysis of pad/surface interaction and induced stresses in thin films and substrate.

- **Effects of slurry chemistry on agglomeration and surface hardness**
  - Investigate effects of heating (temperature) on the agglomeration of the abrasives and the wafer surface hardness as a function of chemistry.