Fundamental Study of Interfacial Phenomena and Modeling for CMP Consumables Design

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Outline

• Part 1: Interfacial Phenomena
  – Lubrication regime
  – CMP interaction
  – Summary

• Part 2: Modeling
  – CMP modeling
  – Application to design of consumables
  – Summary
INTERFACIAL PHENOMENA FOR CMP CONSUMABLES DESIGN
Contact condition

Striebeck Curve

- **A** regime
- **B** regime
- **C** regime

**Viscosity*Velocity/pressure**

**COF**

- Boundary lubrication
- Partial lubrication
- Hydrodynamic lubrication

Sommerfeld number

Boundary lubrication

Mixed lubrication

elastohydrodynamic lubrication

Hydrodynamic lubrication

"A" regime

wafer

pad

abrasive

"B" regime

wafer

pad

abrasive

"C" regime

wafer

pad

abrasive
Wafer-Abrasive-Pad Interaction

1. WAFER
2. ABRASIVE
3. PAD
Wafer-Abrasive-Pad Interaction

(a) without abrasives

(b) with abrasives

Polishing starting with pH 11 solution

End

SiO₂

low friction force

polishing load

pad asperity

SiO₂

high friction force

polishing load

pad asperity

abrasive

RR~100 Å/min

RR~2200 Å/min
Interaction between silica–, ceria abrasive and oxide film surface

silica-based slurry

1. Formation of a little hydrated surface in alkaline slurry
2. Indentation of silica particles on SiO₂ film surface
3. Plastic deformation of SiO₂ film surface with friction force
   Formation of hydrated surface around deformation region
   (Si-O-Si bonds breaking)
4. Simultaneously plowing of abrasive

ceria-based slurry

1. Formation of a little hydrated surface in neutral slurry
2. Indentation of ceria particles on SiO₂ film surface
3. Plastic deformation of SiO₂ film surface with friction force
   Formation of hydrated surface around deformation region
   (Si-O-Si bonds breaking with Ce-O-Si bonding)
4. Simultaneously plowing of abrasive


L. Cook, Journal of Non-Crystalline Solids, 120 (1990), 152-171
Formation of hydrated layer after CMP

Silica-based slurry

Si-O stretching

Si-OH

pH 11

pH 7

pH 2

Absorbance (a.u.)

Wavenumber (cm⁻¹)

Ceria-based slurry

Si-OH

pH 11

pH 7

pH 2

Absorbance (a.u.)

Wavenumber (cm⁻¹)

Low hydration

- Same material

High hydration

- Strong chemical reaction between abrasive and SiO₂ film
The number of abrasive particles played an important role in material removal. The ceria slurry has high MRR efficiency in spite of low abrasive concentration and neutral environment of slurry.
Schematic of active abrasive particles

Microscopic contact in mixed lubrication

Contact at low abrasive concentration

Transition

Contact at high abrasive concentration

- Active abrasive with two-body abrasion
- Active abrasive with three-body abrasion
- Inactive abrasive

Increase of abrasive concentration
Abrasive and Pad Interaction

Down force

Surface topography

Wetted surface layer

Abrasive

Deformed layer

Area of real contact

Slurry

Pad
Basic material removal model

Material removal rate

\[ = \rho_w * N * Vol_{\text{removed}} + C_{\text{chemical action}} \]

\[
\begin{align*}
\rho_w &= \text{material density of wafer (constant)} \\
N &= \text{number of active abrasive} \\
Vol_{\text{removed}} &= \text{volume removed by a single abrasive (constant)} \\
C_{\text{chemical action}} &= \text{material removal amount by chemical (constant)}
\end{align*}
\]

- Active abrasive: cause mechanical material removal
- Asperity distribution of pad means the probability of the number of active abrasive
- Material removal rate \( \propto \) Number of active abrasive \((N)\)
- Real contact area

Histogram analysis of asperity height

- Pad surface topography = peak area + valley area

**Peak area**
- Reaction region (mechanical loading)
- Active layer of pad top layer
- Multiple direct contacts with abrasives
- The most rapid wear during the polishing

**Valley area**
- Space for slurry reservoir
- Ability to retain polishing slurry
Asperity height distribution of conditioned pad

Conditioned pads show variable distribution of asperity height.

- Asperity distribution has a significant effect on material removal behavior during CMP process.

#A > #B > #C > #D

Coarse >>>>>>Fine

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Analysis of area of real contact

As-received pad

Conditioner A

Conditioner B

0.27%

0.89%

1.45%

Randomly distributed asperities

Uniformly distributed asperities

• Pad conditioning process has a strong effect on distribution of pad asperity height.
• High real contact area can ensure stable material removal and low stress planarization.
Analysis of contact angle

1. Contact angle $\propto$ Roughness
Higher roughness value
  > Thicker gap between peak/valley
  > More air trap inside topography

..... Higher contact angle

2. Contact angle $\propto$ Uniformity of Roughness
Randomly distributed asperities
... Higher contact angle

>>>>>
Makes pad more hydrophobic and MRR lower
Analysis of viscoelastic deformation

- Strain: Randomly distributed asperities > uniformly distributed asperities
- Small and uniform deformation = more stable against creep and recovery
- Deformation of asperity layer can be strongly influenced by pad conditioning process regardless of same pad.

Xie, Thesis of Doctor, 2007
Summary and Future Work

- Hydration surface layer
- Definition of active abrasive
- Theoretical approach; simulation and modeling of active abrasive’s behavior
- New abrasive particle for effective material removal

- Uniform distribution of pad asperity
- Theoretical and experimental approach; estimation of active abrasive
- Molding pad; optimization of pad asperity
- Optimization of pad groove design
- Mean residence time of slurry
- Optimization of pad conditioner geometry
- Estimation of active diamond of pad conditioner
- New pad for emerging hard and soft material such as compound semiconductor
- Simulation of slurry flow including abrasive

- Free abrasive processing
  - Not significant
- Fixed abrasive pad
  - Significant
  - Optimization of FAP geometry
  - Modeling of MRR
MODELING FOR CMP CONSUMABLES DESIGN
Seungchoun Choi, Shantanu Tripathi, Fiona Doyle and David Dornfeld
Mechanistic model for copper CMP

1. Passivation kinetics: the transient oxidation rate of copper after removal of passive film

2. Mechanical response of passive films

3. Abrasive-copper interaction frequency & force

All three components need to be individually estimated for modeling
Copper CMP Material Removal Model

Passivation kinetics
- Film growth kinetics

Mechanical removal response of passive film

Asperity-abrasive-copper interaction force and frequency

Oxidation rate $\text{mA/cm}^2$ vs. Time ($t'$) ms

Bare copper

Copper: transient passivation behavior $i(t')$

$t_0$ can be found given $L(t')$ (fig 1.), $\Delta L$ (fig 2.) & $\tau$ (fig 3.) (since $L(t')$ is concave)

Passive Film Thickness (L) (nm)

Film thickness removed, $\Delta L$ Å

Integral for Removal Rate ($RR$)

Removal Rate ($RR$) $= \frac{M_{Cu}}{\rho n F \tau} \int_{0}^{\tau} i(t_0 + t) dt$

$t_0$

Force (nN) vs. Time (ms)

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

Mechanical removal response of passive film

Atomic mass of copper $M_{Cu}$

Density of copper $\rho$

Number of electrons transferred $n$

Faraday’s constant $F$

Asperity-abrasive-copper interaction force and frequency

CMPUG • 21
Input Parameters for Model

**Frequency of Mechanical Interactions**

- Elmufdi and Muldowney (2006) have measured the real contact area of asperities on a typical commercial pad using confocal reflectance interference contrast microscopy.
- Real contact ratio, $Ar\%$, between 1 and 10% for the usual operating CMP pressures.
- Where $Ar\%$ was 1%, the average asperity contact area, $\overline{Asp_{area}}$, was about 100 $\mu m^2$.
- If relative pad-wafer velocity is 1 m/s, then average interval between consecutive asperity-copper contacts:

$$\tau = \frac{\sqrt{Asp_{area}}}{V \cdot Ar\%} = 1 \text{ ms}$$

- Duration of contact:

$$\sqrt{\frac{Asp_{area}}{V}} = 10 \mu s \ll 1 \text{ ms}$$

sum abrasive-Cu and asperity-Cu contacts
Protective Film Formed on Cu Surface During Cu CMP in Acidic Slurry Containing BTA

- For intervals between two asperity copper contacts of 1 to 10ms, this corresponds to removal of a copper layer of 0.1 to 1Å thick per interaction => less than one atomic layer of copper (1.4Å)
- Removal due to both dissolution between the two interactions and removal of oxidized copper film by the interaction
- Typical copper removal rates during CMP are in the range of 50 to 600 nm/min.

- There exists only a portion of monolayer protective film on copper during CMP in acidic slurries containing BTA
- A portion of the protective material is removed by the action of asperities/abrasives

![Chronoamperometry result](image)

[Tripathi, 2008]
Removal of Protective Film During CMP

- The coverage ratio, $\Theta$ is reduced by asperities/abrasives-copper interactions (equivalent to the film thickness reduction where thicker film is formed)

- Removal efficiency:

$$e = 1 - \frac{\theta_{\text{after removal}}}{\theta_{\text{before removal}}}$$

- Determined by duration of contact between the material being removed and asperity/abrasives and the material properties of pad, abrasives and the material being removed

\[ \theta_{\text{Bare copper surface}} = 0.16 \]
\[ \theta_{\text{Chemisorbed BTA on copper (Cu(I)BTA)}} = 0.84 \]
\[ e = 0.2 \]
### Implications for Design of Consumables

- Draw principal consumables design parameters from the model

<table>
<thead>
<tr>
<th>Principal design parameters</th>
<th>Interval between consecutive copper-asperity contacts (τ)</th>
<th>Removal efficiency, e</th>
<th>Passivation kinetics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pad Design</td>
<td>Adjusting distance between asperities and pad compliance*</td>
<td>Adjusting pad compliance and material properties</td>
<td>-</td>
</tr>
<tr>
<td>Abrasive Design</td>
<td>-</td>
<td>Varying abrasive concentrations, size or materials</td>
<td>-</td>
</tr>
<tr>
<td>Slurry Design</td>
<td>-</td>
<td>-</td>
<td>Varying slurry chemistry</td>
</tr>
</tbody>
</table>

* same effect can be obtained by adjusting processing parameters such as applied pressure and rotational speeds
Implications on Pattern Dependence of Copper CMP

- MRR discrepancy by step height

More abrasives & higher pressure ~ higher e
Less abrasives & lower pressure~ lower e

- MRR discrepancy by different materials being removed

Different removal efficiency, e
Different interaction interval, \( \tau \)

Different removal efficiency, e
Different passivation kinetics
Summary

• Copper CMP model developed here recognizes principal consumables design parameters, namely passivation kinetics, removal efficiency, $\epsilon$ and asperity-copper interaction interval $\tau$
• Pattern related defects can be accounted for and potentially be addressed by these design parameters

Future Work

• To identify factors that affect removal efficiency for Cu in various slurry chemistries
• To develop pattern dependence model by incorporating developed material removal model
Acknowledgement

• Part 1: Interfacial Phenomena

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• Part 2: Modeling

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