Update: Brush Scrubbing for Post-CMP Cleaning

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Environmentally-Benign Semiconductor Manufacturing

Existing Manufacturing Processes

- New materials
- New processes

Fundamental science

Process models

New Manufacturing Processes

Optimal Manufacturing Processes

Reduced Waste

Reduced Energy

Benign Waste

ASU
Chemical Mechanical Polishing (CMP)

- Removes a thin surface layer to obtain planar wafers
  - Uses abrasive particles in aqueous solution in conjunction with relative motion between polishing pad and wafer
  - Surface removed mechanically and chemically
- Introduces contaminants onto wafer surfaces
  - Pieces of polished surface and polishing pad
  - Slurry particles
  - Contamination from the handler or handling device
  - Must be removed before further processing
Post-CMP Cleaning

» Must remove particles less than 1 micron in diameter
» Must not roughen wafer surface excessively
» Brush scrubbing and megasonic cleaning have potential for removing small particles
» Problems with
  • Resource consumption
  • Lack of understanding of cleaning mechanism
  • Inefficient and unreliable processes

**Brush Scrubber**

- Cleaning Solution
- Wafer Holder
- PVA Brush

\[ r = \text{radius} \]
\[ \omega = \text{angular speed} \]
Cleaning Model Objective

Develop and validate scientifically-based cleaning models to optimize wafer cleaning processes and minimize water and chemistry use.

1st Generation
Rough deformable spherical particles interacting with a rough flat surface

2nd Generation
Asymmetrical rough particles interacting with real surfaces

Adhesion Model

Removal Model

Particle size variation
Adhesion force variation
Points around which rolling occurs
Velocity profile near adhering particle
Adhesion of Particles to Surfaces – DLVO Theory

\[ F_A = F_{\text{vdW}} + F_{\text{EDL}} \]

**Total Adhesion Force**

- \( F_{\text{vdW}} = f(A, d, a, h) \)
- \( F_{\text{EDL}} = f(\varepsilon, \zeta, \kappa, d, h) \)

\[ A = \text{System Hamaker constant} \]
\[ d = \text{Particle diameter} \]
\[ a = \text{Contact radius} \]
\[ h = \text{Particle-surface separation distance} \]
\[ \varepsilon = \text{Medium dielectric constant} \]
\[ \zeta = \text{Zeta potential} \]
\[ \kappa = \text{Reciprocal double-layer thickness} \]
\[ I = \text{Medium ionic strength} \]

**Diagram:**
- Particle
- Surface
- Hamaker constant
- Contact radius
- Particle-surface separation distance
- Dielectric constant
- Zeta potential
- Reciprocal double-layer thickness
- Medium ionic strength

**Note:**
- The diagram illustrates the interaction between a particle and a surface, showing the forces involved in adhesion.
- The forces are decomposed into van der Waals forces and electrostatic double-layer forces, each dependent on specific parameters.
Adhesion of Particles to Surfaces – Real Systems

\[ F_A = F_{\text{vdW}}(A, h, E, P, f_s, \varepsilon_s, \sigma, f_p, \varepsilon_p, \sigma_p, a, d) \]

\begin{itemize}
  \item $A$ = System Hamaker constant
  \item $h$ = Particle-surface separation distance
  \item $E$ = Elastic modulus
  \item $P$ = Applied load
  \item $f_s$ = Fraction of substrate covered by asperities
  \item $\varepsilon_s$ = Average asperity height on substrate
  \item $\sigma_s$ = Standard deviation in asperity height on substrate
  \item $f_p$ = Fraction of particle covered by asperities
  \item $\varepsilon_p$ = Average asperity height on particle
  \item $\sigma_p$ = Standard deviation in asperity height on particle
  \item $a$ = Contact radius
  \item $d$ = Particle diameter
\end{itemize}
Adhesion Model – Gen 2

» Predicts adhesive interactions for particles on various surfaces
  • Couples computer simulation with fundamental adhesion model
  • Accounts for particle and surface:
    › Chemistry
    › Morphology
    › Mechanical properties
    › Geometry

» Validated using experimental investigations of adhesion of alumina particles and polystyrene latex spheres to copper, SiO₂, and tungsten substrates in a variety of environments
  • Atomic force microscopy (AFM), nanoindentation, and scanning electron microscopy (SEM) techniques applied
    › Measure force required to remove particles from the substrates
    › Characterize morphology, mechanical properties, and geometry of interacting surfaces
  • Experimental removal forces compared with model predictions
  • Measurements can be used to determine system Hamaker constant

» Predictive model for particle adhesion established
PSL/H₂O/Silicon Adhesion

PSL particles in contact with a silicon substrate in water

- Experimental Data (average of 50 measurements)
- Model Predictions (average of 5000 predictions)

Removal Force = Adhesion Force

\[ \text{Particle Radius (\(\mu\text{m}\))} \]

\[ \text{Removal Force (nN)} \]
Alumina/H$_2$O/Silicon Adhesion

3 µm alumina particle (contact radius = 350 nm) in contact with a silicon substrate in DI H$_2$O

Average Observed Force = 176 nN

Range of Observed Force = 139 - 201 nN

Removal Force = Adhesion Force
Substrate, Media Effects: Alumina Adhesion

- Experimental Data
- Ideal vdW Prediction
- Average Simulation Prediction
- Range of Simulation Prediction (+/- σ)

Removal Force = Adhesion Force

Removal Force (nN)

- Al₂O₃/N₂/SiO₂ System
- Al₂O₃/H₂O/SiO₂ System
- Al₂O₃/N₂/Cu System
- Al₂O₃/H₂O/Cu System
Removal Model Objective

Assess mechanism(s) of micron-scale particle removal from semiconductor wafer surfaces using a critical particle Reynolds number approach

- Relate adhesion models to particle removal
- Relate flow characteristics to particle removal
- Develop model for removal processes by combining adhesion and flow models
Removal Model Validation


• Studied detachment of spherical glass particles from a flat glass surface
• Used laminar channel flow over a range of flow rates to remove adhering particles
• Percentage adhering as a function of wall shear stress ($\tau_w$) presented graphically
• System Properties
  ‥ Fluid: solution of distilled water, HNO$_3$, and NaNO$_3$
  ‥ Particle (mean) diameters: 2, 5, 10, 15 µm ($\sigma_d \sim 12\%$)
Particle Adhesion/Removal Model

\[ \mu = \frac{\rho V_p}{\mu} \]

\[ F_A = \text{Gen 2 adhesion force} \]
\[ F_L = \text{Lift force} \]
\[ M_D = \text{External moment} \]
\[ F_D = \text{Drag force} \]

Points around which rolling can occur.
Rolling Particle Removal Criteria

\[ \tilde{M}_R (\tilde{M}_D, \tilde{F}_D, \tilde{F}_L, l_1, l_2) \geq \tilde{M}_A (\tilde{F}_A, l_2) \]

- External moment of surface stresses about center of particle
  \[ M_D \propto d \text{Re}_p \]
  - Drag force
    \[ F_D (\text{Re}_p < 1) \propto \text{Re}_p \]
    \[ F_L \propto d \frac{du}{dz} \text{Re}_p \]
  - Lift force
  - Adhesion force
  \[ F_A \propto Ad \]
- Vertical lever arm
  \[ l_1 (d, a, \alpha, \varepsilon_1) \]
- Horizontal lever arm
  \[ l_2 (d, l_1) \]
Assessing Particle Removal

» Removal occurs when $\text{Re}_p(\text{Flow}) \geq \text{Re}_{pc}(\text{Rolling})$

$\text{Re}_p(\text{Flow})$ constant at constant flow rate (for this system)

» \textbf{Ideal system} of smooth, deformable spherical particles of identical radius adhering to a smooth, flat, deformable surface

→ Single adhesion force

⇒ Single value of $\text{Re}_{pc}$

⇒ All or none of the adhering particles should be removed

» \textbf{Real system} of deformable particles with non-uniformly distributed roughness and a finite size distribution adhering to a deformable surface with a non-uniform roughness distribution

→ Multiple adhesion forces and multiple points around which rolling can occur

⇒ Multiple values of $\text{Re}_{pc}$

⇒ All, some, or none of the adhering particles can be removed
Adhesion Profile – Ideal System, $d = 2$ and $15 \, \mu m$

$\tau_w \propto Q \, (cm^3/s)$

$\tau_w$ – Wall Shear Stress, $Q$ – Flow Rate
Effect of Roughness on $\text{Re}_{pc}$

Roughness affects $\text{Re}_{pc}$ by affecting
- Adhesion force
- Point around which rolling can occur

Length of horizontal and vertical lever arms ($l_1$ and $l_2$) depend on $\varepsilon_1$
Removal Analysis Procedure

Particle, Surface, and System Characteristics
\[ A, h_{L,p}, E, P, f_s, \varepsilon_s, \sigma_s, f_p, \varepsilon_p, \sigma_p, \alpha \]

Gen 2 Adhesion Force Distribution

Re_{pc\text{(Rolling)}} Distribution
- Particle Size Variation
- Adhesion Force Variation
- Points Around which Rolling Occurs

Velocity Profile
- \[ V_p, du/dz \]

Re_p(Flow)

Percentage Adhering/Removed
Adhesion Profile – Real System, $d_{\text{mean}} = 2 \, \mu\text{m}$

$\tau_w \propto Q \, (\text{cm}^3/\text{s})$

Yiantsios and Karabelas, $t = 4\, h$
Yiantsios and Karabelas, $t = 8\, h$
Prediction, $A = 6.8 \times 10^{-20} \, \text{J}$
Adhesion Profile – Real System, $d_{\text{mean}} = 15 \, \mu m$

Yiantsios and Karabelas Prediction, $A = 6.8 \times 10^{-20} \, J$

$$\tau_w \propto Q \, (\text{cm}^3/\text{s})$$
Removal Model Conclusions

» Accurate particle removal models require accurate particle adhesion models

» Rolling is the controlling removal mechanism

» Roughness and particle size distribution affect the point around which rolling can occur

» (Rolling) theoretical adhesion profiles for real adhesion system in agreement with those of Yiantsios and Karabelas

» Critical particle Reynolds number approach validated

» Predictive model for particle removal established

   Independent of particle size and cleaning (flow) system
Brush Scrubbing Analysis Objective

Use critical particle Reynolds number ($Re_{pc}$) approach to assess particle removal from wafer surfaces during brush scrubbing.

Typical Operating Conditions
- $\omega_B = 200$ rpm $\omega_w = 90$ rpm
- $r_{cc} = 5$ cm $r_B = 5.7$ cm
- Total cleaning time, $t$: 20 s
- Brush Pressure, $P_B$: 3 psi
- Finger diameter, $d_f$: 0.6 cm
- Number of fingers per brush, $N_f$: 85
- Total area covered by fingers: 66,000 cm$^2$

System Properties
- Particles: asymmetrical alumina
- Surfaces: polished silicon dioxide and copper

$r$ = radius
$\omega$ = angular speed
Brush Scrubbing Analysis Objective, cont’d

» Assess whether hydrodynamic forces can remove adhering particles from wafer surfaces during brush scrubbing, or whether brush-particle contact must occur
  • Systems of 0.1 and 1.0 µm diameter alumina particles adhering to polished silicon dioxide and copper surfaces considered
  • Two approaches: time-dependent and time-averaged

» Calculate particle Reynolds numbers as a function of
  • Time (t)
  • Brush radial position (r)
  • Brush-wafer separation distance (D)
  • Brush and wafer angular speed (ω_B and ω_w)

» Consider the effects of
  • Substrate chemistry
  • Particle and substrate morphology and mechanical properties
  • Geometry of the interacting surfaces
  • Fluid properties
  • Velocity profile near adhering particle
Velocity Profile

» Two approaches
  • Use time-dependent relative velocity ($V_{rel}$) to calculate $V_p$ and $Re_p$
  • Use time-averaged relative velocity ($V_{rel}$) to calculate $V_p$ and $Re_p$

» Calculate boundary layer thickness ($\delta$) on brush finger
  • Determines relationship between $V_p$, $V_{rel}$, and $D$
  • If $D \leq \delta$:
    \[
    V_p = \frac{|V_{rel}|}{D} \cdot \frac{d}{2} \quad Re_p = \frac{\rho \cdot |V_{rel}|}{\mu} \cdot \frac{D \cdot d^2}{2}
    \]
Time-Dependent Velocity Profile

![Graph of Time-Dependent Velocity Profile](#)
Time-Averaged Velocity Profile

![Graph showing time-averaged velocity profile vs. brush radial position (r cm).](chart.png)
Time-Dependent Boundary Layer Thickness
Time-Averaged Boundary Layer Thickness

[Graph showing the relationship between Boundary Layer Thickness (mm) and Brush Radial Position (r cm).]
# System Properties

<table>
<thead>
<tr>
<th>Particle size (µm)</th>
<th>Contact Radius, a (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>22.6</td>
</tr>
<tr>
<td>1.0</td>
<td>226</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Al₂O₃ Particle</th>
<th>SiO₂</th>
<th>Cu</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average asperity height, ε (nm)</td>
<td>1.6</td>
<td>1.7</td>
<td>0.8</td>
</tr>
<tr>
<td>Standard deviation in asperity height, σ (nm)</td>
<td>0.7</td>
<td>0.7</td>
<td>0.5</td>
</tr>
<tr>
<td>Fraction of surface covered in asperities, f</td>
<td>0.33</td>
<td>0.56</td>
<td>0.45</td>
</tr>
<tr>
<td>Elastic modulus, E (N/m²)</td>
<td>$5.0 \times 10^{11}$</td>
<td>$5.6 \times 10^{11}$</td>
<td>$7.8 \times 10^{10}$</td>
</tr>
</tbody>
</table>
Al$_2$O$_3$-H$_2$O-SiO$_2$ Adhesion Force

1.0 µm alumina particle adhering to polished silicon dioxide in deionized water

\[ \sigma_A = 1.2 \text{ nN} \]
Al₂O₃-H₂O-Cu Adhesion Force

1.0 µm alumina particle adhering to copper in deionized water

\[ \sigma_A = 9.6 \text{ nN} \]
Al$_2$O$_3$-H$_2$O-SiO$_2$ Critical Particle Reynolds Number

Re$_{pcmean} = 0.0010$
$\sigma_{Re} = 0.00048$

Re$_{pcmean} = 0.089$
$\sigma_{Re} = 0.042$

0.1 µm alumina particle adhering to polished silicon dioxide in deionized water

1.0 µm alumina particle adhering to polished silicon dioxide in deionized water
Al₂O₃-H₂O-Cu Critical Particle Reynolds Number

Re_{pcmean} = 0.0096
σ_{Re} = 0.0036

Re_{pcmean} = 0.91
σ_{Re} = 0.33

0.1 µm alumina particle adhering to copper in deionized water

1.0 µm alumina particle adhering to copper in deionized water
Analysis Algorithms

**Time-Dependent**

1. Calculate $|\bar{V}_{rel}(t,r)|$
2. Calculate $Re_p(V_{rel}(t,r),D)$
3. Set $Re_{pc}$ distribution, $Re_{pc}(i) = Re_{pc}(\text{mean}) + i\sigma$
   $(i = 0, \pm1, \pm2, \pm3, \sigma = \text{standard deviation})$
4. Calculate the fraction ($R$) of $Re_p$ greater than $Re_{pc}$ over a given interval ($\sigma$) using $^\dagger$
   \[
   R(i,i+1) = \frac{\int_{t_0}^{t}[\{(Re_p(t,r,D) - Re_{pc}(i)) - (Re_p(t,r,D) - Re_{pc}(i+1))\}]dt}{\int_{t_0}^{t}\sigma dt}
   \]
5. Calculate the percentage of particles removed using
   \[
   \% \text{ Removed} = \sum_i R(i,i+1) \cdot F(i,i+1)
   \]
   where $F$ is the frequency (%) from the $Re_{pc}$ distribution

**Time-Averaged**

1. Calculate $\bar{V}_{rel}(r)$
2. Calculate $Re_p(V_{rel}(r),D)$
3. Compare $Re_p$ with the $Re_{pc}$ distribution and calculate the percentage of particles removed

$^\dagger$ Integral in numerator calculated only for the time when $Re_p > Re_{pc}$
Time-Dependent Analysis – Example, $r = 2.85$ cm

1.0 $\mu$m alumina particle adhering to polished silicon dioxide in deionized water

\[
D = d = 1.0 \ \mu m
\]

<table>
<thead>
<tr>
<th>i,i+1</th>
<th>$R(i,i+1)$</th>
<th>$F(i,i+1)$</th>
<th>$R(i,i+1) \cdot F(i,i+1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-3,-2</td>
<td>1.0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>-2,-1</td>
<td>1.0</td>
<td>18.37</td>
<td>18.37</td>
</tr>
<tr>
<td>-1,0</td>
<td>0.98</td>
<td>32.65</td>
<td>32.00</td>
</tr>
<tr>
<td>0,1</td>
<td>0.86</td>
<td>28.57</td>
<td>24.57</td>
</tr>
<tr>
<td>1,2</td>
<td>0.78</td>
<td>20.41</td>
<td>15.92</td>
</tr>
<tr>
<td>2,3</td>
<td>0.70</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

$\%$ Removed = $\sum_i R(i,i+1) \cdot F(i,i+1)$ = 91

$R =$ fraction of $R_{ep}$ greater than $R_{pc}$ over a given interval

$F =$ frequency (%) from $R_{pc}$ distribution
Time-Averaged Analysis – Example, \( r = 2.85 \) cm

1.0 \( \mu \)m alumina particle adhering to polished silicon dioxide in deionized water

\[
\text{Frequency (\%)} \quad \text{Re}_p (D = d = 1.0 \ \mu \text{m}) \\
\text{All of the particles removed}
\]

\[
\text{Re}_p (D = 10 \ \mu \text{m}) \\
\sim 9\% \text{ of the particles removed}
\]
Silicon Dioxide Removal Profiles, \( d = 0.1 \ \mu m \)

0.1 \( \mu m \) alumina particles adhering to polished silicon dioxide in deionized water

- **Time-averaged**
- **Time-dependent**

\[ A = 6.2 \times 10^{-20} \ \text{J} \]
Silicon Dioxide Removal Profiles, \( d = 1.0 \, \mu m \)

1.0 \( \mu m \) alumina particles adhering to polished silicon dioxide in deionized water

![Graph showing percent removed vs brush radial position for different particle sizes.

- **Time-averaged**
- **Time-dependent**

Brush-particle contact must occur for complete particle removal

\[ A = 6.2 \times 10^{-20} \, J \]
Copper Removal Profiles, $d = 0.1 \, \mu m$

0.1 \, \mu m alumina particles adhering to copper in deionized water

Time-averaged

Time-dependent

Brush-particle contact must occur for complete particle removal

$D = 0.1 \, \mu m$

$D = 10 \, \mu m$

$A = 6.2 \times 10^{-20} \, J$
Copper Removal Profiles, \(d = 1.0 \, \mu m\)

1.0 \(\mu m\) alumina particles adhering to copper in deionized water

Time-averaged

Time-dependent

Brush-particle contact must occur for complete particle removal

\[
A = 6.2 \times 10^{-20} \, \text{J}
\]
Brush Scrubbing Analysis Conclusions

» Under limited conditions (i.e., particle size, brush radial position, and brush-wafer separation distance), the time-averaged analysis predicts almost identical results to the time-dependent analysis.

» Time-averaged analysis predicts that as brush radial position increases and brush-wafer separation distance decreases, the percentage of particles removed increases.

» Time-dependent analysis predicts that as brush-wafer separation distance decreases, the percentage of particles removed increases, but follows no overall trend as a function of brush radial position.
Brush Scrubbing Analysis Conclusions, cont’d

» Based on mechanics alone more particles are expected to be removed from the silicon dioxide surface than from the copper surface since the copper system has a larger $\text{Re}_{pc}$ under the same flow conditions

» In many cases brush-particle contact must occur for complete particle removal

» Larger particles are more difficult to remove
  • $\text{Re}_p$ and $F_A$ both proportional to $d^2$, therefore contact radius controls the level of difficulty in removing a particle
  • Larger particles, having a larger contact radius, are more difficult to remove since there is more mass interacting at the particle-wafer interface than for smaller particles
  • $\text{Re}_p$ must increase proportionally to remove these particles

» Hydrodynamic particle removal is system dependent
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