Diagnostics of the plasma-surface interface: coupling experiments with simulations

A. Greb\textsuperscript{1}, A. R. Gibson\textsuperscript{2}, K. Niemi\textsuperscript{1}, D. O’Connell\textsuperscript{1}, T. Gans\textsuperscript{1}

\textsuperscript{1} York Plasma Institute, Department of Physics, University of York, UK
\textsuperscript{2} Centre for Plasma Physics, Queen’s University Belfast, UK
Motivation

Understanding the dynamics of plasma-surface interface

Key importance:
- Determination of surface condition
- Measurement of important reactive species (e.g. atomic oxygen)

Most promising approach: Coupling of optical diagnostics and simulations

Advanced Real-Time Process Control & Monitoring
Experimentally Benchmarked Fluid Model [1]

- Experimental setup as foundation for model
  - Capacitively Coupled Oxygen Discharge
  - Geometric asymmetry
  - RF power input at 13.56 MHz
  - DC bias voltage (calculated self-consistently based on flux balance)
  - 40 mm electrode gap, typical operation pressures: 10 – 100 Pa (~100 – 1000 mTorr)

- Includes electron dynamics & simple plasma chemistry
  - Considered species: e, O₂, O₂⁺, O⁻, O₂(¹Δ)
  - Improved ion mobility treatment
  - Iterative multi-scale modelling approach

Simulation: Impact of Surface Conditions

- Consider important surface reaction mechanisms:
  - Surface neutralisation
  - $O_2(^1\Delta)$ surface loss probability
  - Secondary electron emission
    - Induced by $O_2^+$ ions

<table>
<thead>
<tr>
<th>Electron density</th>
<th>$O_2(^1\Delta)$ density</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct impact</td>
<td>$O_2^+ / O^-$ densities</td>
</tr>
<tr>
<td>Impact on charged particles</td>
<td>Excitation mechanisms</td>
</tr>
</tbody>
</table>

- Actual surface condition determines how much $O_2(^1\Delta)$ is neutralised.
Experiment: Excitation Dynamics ($\lambda = 844$ nm)

- **Teflon wafer [2]**
  - Two excitation features present
    - Sheath expansion excitation (I)
    - Sheath collapse excitation (II)
  - (II) more pronounced than (I)

---

Experiment: Excitation Dynamics \((\lambda = 844\ \text{nm})\)

- Stainless steel wafer [2]
  - Two excitation features present
    - Sheath expansion excitation (I)
    - Sheath collapse excitation (II)
  - Change in prominence and shape

Experiment (Stainless steel)

Simulation (Stainless steel)

List of Investigated Materials

- Experimental condition:
  - Oxygen plasma
  - 40 Pa, 300 V, 13.56 MHz, 40 mm gap

<table>
<thead>
<tr>
<th>Wafer material</th>
<th>SDO surface loss probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stainless Steel</td>
<td>$1 \times 10^{-5}$</td>
</tr>
<tr>
<td>Tungsten</td>
<td>$1 \times 10^{-5}$</td>
</tr>
<tr>
<td>Aluminium</td>
<td>$6 \times 10^{-5}$</td>
</tr>
<tr>
<td>Gold</td>
<td>$6 \times 10^{-5}$</td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>$1 \times 10^{-4}$</td>
</tr>
<tr>
<td>Copper</td>
<td>$2 \times 10^{-4}$</td>
</tr>
<tr>
<td>Silicon</td>
<td>$4 \times 10^{-4}$</td>
</tr>
<tr>
<td>Teflon</td>
<td>$3 \times 10^{-3}$</td>
</tr>
</tbody>
</table>
Work Function Analysis

- **Theory:**
  - High SE emission for low material work function

$$\gamma_{se} \approx 0.016 (\epsilon_{i,iz} - 2\epsilon_{\Phi})^*$$
  
  if $\epsilon_{i,iz} > 2\epsilon_{\Phi}$

Secondary electron emission coefficient

- **Experiment:**
  - Use best defined materials
  - Qualitative comparison of excitation signal

- **Confirmation of theoretical assumption**
  - Qualitative comparison as benchmark for other materials
## Combined results for investigated wafer materials

<table>
<thead>
<tr>
<th>Wafer material</th>
<th>SDO surface loss probability</th>
<th>Secondary electron emission coefficient (by O$_2^+$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stainless Steel</td>
<td>$1 \times 10^{-5}$</td>
<td>$\approx 0.030$</td>
</tr>
<tr>
<td>Tungsten</td>
<td>$1 \times 10^{-5}$</td>
<td>$\approx 0.043$</td>
</tr>
<tr>
<td>Aluminium</td>
<td>$6 \times 10^{-5}$</td>
<td>$0.060 \pm 0.003$</td>
</tr>
<tr>
<td>Gold</td>
<td>$6 \times 10^{-5}$</td>
<td>$0.020 \pm 0.002$</td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>$1 \times 10^{-4}$</td>
<td>$\approx 0.040$</td>
</tr>
<tr>
<td>Copper</td>
<td>$2 \times 10^{-4}$</td>
<td>$\approx 0.040$</td>
</tr>
<tr>
<td>Silicon</td>
<td>$4 \times 10^{-4}$</td>
<td>$0.036$</td>
</tr>
<tr>
<td>Teflon</td>
<td>$3 \times 10^{-3}$</td>
<td>$\approx 0.0$</td>
</tr>
</tbody>
</table>
Conclusions

- Plasma dynamics can change surface condition (e.g. etching, deposition)
- Surface condition governs plasma parameters & dynamics

Synergistic coupling of simulations and measurements is key for development of Real-Time Metrology.
Thank you!