PLASMA EQUIPMENT MODELING FOR PROCESS DESIGN*

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• Goals and requirements for Plasma Equipment and Process Modeling

• A "Walk-Through" of plasma properties for ICP conductor etching.

• Overview of Modeling Hierarchy

• Profile Control for Etching and Deposition

• Concluding Remarks
The majority of the processes which enable fabrication of advanced interconnect structures are based on plasma processing (etching, deposition, cleaning).
• Plasmas play a dual role in microelectronics fabrication...

• First, electron impact on otherwise unreactive gases produces neutral radicals and ions. That is, electrons are a power transfer medium.

\[ e + CF_4 \rightarrow CF_3^+ + F + 2e \]
\[ \rightarrow CF_2 + 2F + e \]

• These active species drift or diffuse to the wafer where they remove or deposit materials.

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Second, ion acceleration in sheaths delivers directed activation energy to surfaces which enables fine features to be fabricated having extreme and reproducible tolerances.

- Ion Assisted Etching
- Neutral Dominated Etching

0.25 μm Feature (C. Cui, AMAT)
MOTIVATION FOR PLASMA EQUIPMENT/PROCESS MODELING

• As fab construction costs increase well beyond $1 Billion, a larger proportion of the costs are consumed by processing equipment.

• The motivation for plasma equipment and process modeling is then:
  • Reduce the cost of developing equipment and processes.
  • Increase utilization of equipment to address multiple processes.
The typical low pressure (<10s - 100s mTorr) plasma processing reactor is powered by inductive and capacitive coupling, and may have auxiliary static magnetic fields.
The general properties of an Ar/Cl\textsubscript{2} inductively coupled plasma tool will be examined.

The inductively coupled electromagnetic fields have a skin depth of 3-4 cm.

Absorption of the fields produces power deposition in the plasma.

Electric Field (max = 6.3 V/cm)

Ar/Cl\textsubscript{2} = 80/20

20 mTorr

1000 W ICP

250 V bias, 2 MHz (260 W)
**Ar/Cl\(_2\) ICP TOOL: POWER AND ELECTRON TEMPERATURE**

- Power deposition from the inductive fields results in electron heating.
- At 2 MHz, power from the capacitive fields produces ion acceleration with little electron heating.

**Power Deposition** (max = 0.91 W/cm\(^3\))

**Electron Temperature** (max = 5 eV)

**Ar/Cl\(_2\) = 80/20, 20 mTorr, 1000 W ICP, 250 V, 2 MHz bias (260 W)**

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AMATET_0500_10
Ar/Cl$_2$ ICP TOOL: IONIZATION

- Electron impact ionization by the bulk electrons heated by the inductively coupled fields dominates.
- Ionization by sheath accelerated beam electrons is less important due to their long mean-free-paths at the low operating pressure.

**Beam ionization** (max = $1.3 \times 10^{14}$ /cm$^3$-s)

**Bulk ionization** (max = $5.4 \times 10^{15}$ /cm$^3$-s)

- Ar/Cl$_2$ = 80/20, 20 mTorr, 1000 W ICP, 250 V, 2 MHz bias (260 W)
• The diffusion of plasma from the remote sources produces a fairly uniform positive ion density in the vicinity of the substrate.

• In general, better uniformity is obtained with a bias than without.

• \( \text{Ar/Cl}_2 = 80/20, \ 20 \text{ mTorr, 1000 W ICP, 250 V, 2 MHz bias (260 W)} \)
**Ar/Cl\textsubscript{2} ICP TOOL: BIAS CURRENTS, POTENTIALS**

- The small current collection area of the substrate produces a large negative dc bias.
- The large sheath potential results in electron current being collected during a small fraction of the rf cycle.
- The non-linearity of the sheaths at different surfaces also contributes to the non-sinusoidal current.
- \(\text{Ar/Cl}_2 = 80/20, 20 \text{ mTorr, 1000 W ICP, 250 V, 2 MHz bias (260 W)}\)

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PHYSICS TO BE ADDRESSED

- GAS INJECTORS (fluid dynamics)
- BULK PLASMA (plasma hydrodynamics, kinetics, chemistry, electrostatics, electromagnetics)
- SOLENOID (magnetostatics)
- COILS (electromagnetics)
- DOME (surface chemistry, sputter physics)
- rf BIASED SUBSTRATE
- POWER SUPPLY (circuitry)
- POLYMER (surface chemistry, sputter physics)
- Secondary emission (beam physics)
- E-FIELD (sheath physics)
- PROFILE EVOLUTION (surface chemistry, sputter physics, electrostatics)

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SPATIAL SCALES IN PLASMA PROCESSING SPAN MANY ORDERS OF MAGNITUDE

- EQUIPMENT SCALE (cm - 10s cm)
  - Gas Flow
  - Heat Transfer
  - Plasma Transport
  - Chemical Kinetics

- FEATURE SCALE (10s nm - µm)
  - Electron, Ion, Radical Transport
  - Plasma Surface Interaction
  - Surface chemistry

- "TRANSITION SCALE" (10s -100s µm)
  - Electron and Ion Transport
  - Sparse Collisions
  - Electrodynamics

\[ e + CF_4 > CF_3^+ + F + 2e \]

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REQUIREMENTS TO MEET MODELING GOALS

• Robust, geometrically flexible simulator to address a wide range of tool types and operating conditions.

• Sufficient dynamic range in space and time to resolve phenomena of interest.

• Databases of fundamental atomic and molecular data to for process relevant chemistries.

• Understanding of limits and proper uses of modeling so that expectations and return-on-investment are realistic.
The wave equation is typically solved in the frequency domain:

\[-\nabla \left( \frac{1}{\mu} \nabla \cdot \vec{E} \right) + \nabla \cdot \left( \frac{1}{\mu} \nabla \vec{E} \right) = \frac{\partial^2 (\varepsilon \vec{E})}{\partial t^2} + \frac{\partial (\sigma \vec{E} + \vec{J})}{\partial t} \]

\[
\vec{E}(\vec{r}, t) = \vec{E}'(\vec{r}) \exp(-i(\omega t + \phi(\vec{r})))
\]

With static applied magnetic fields, conductivities are tensor quantities:

\[
\sigma^* = \sigma_0 \frac{mv_m}{q\alpha} \frac{1}{(\alpha^2 + |\vec{B}|^2)} \begin{pmatrix}
\alpha^2 + \beta_r^2 & \alpha \beta_Z + \beta_r \beta_\theta & -\alpha \beta_\theta + \beta_r \beta_Z \\
-\alpha \beta_Z + \beta_r \beta_\theta & \alpha^2 + \beta_\theta^2 & \alpha \beta_r + \beta_\theta \beta_Z \\
-\alpha \beta_\theta + \beta_r \beta_Z & -\alpha \beta_r + \beta_\theta \beta_Z & \alpha^2 + \beta_Z^2
\end{pmatrix}
\]

\[
\vec{j} = \sigma^* \cdot \vec{E}
\]

\[
\alpha = \frac{(i\omega + v_m)}{q/m}, \quad \sigma_0 = \frac{q^2 n_e}{mv_m}
\]

Circuit models are used to provide antenna currents.
Under conditions where collisional heating and diffusive transport dominate, electron transport coefficients and electron impact source functions are obtained by solving the electron energy equation.

\[
\frac{\partial}{\partial t} \left( \frac{3}{2} n_e k T_e \right) = S(T_e) - L(T_e) - \nabla \cdot \left( \frac{5}{2} \Phi k T_e - \kappa(T_e) \nabla T_e \right) + S_{EB}
\]

where

- \( S(T_e) = \) Power deposition
- \( L(T_e) = \) Electron power loss due to collisions
- \( \Phi = \) Electron flux
- \( \kappa(T_e) = \) Electron thermal conductivity
- \( S_{EB} = \) Electron source from beam electrons

Transport coefficients are obtained as a function of average energy (\( \epsilon = (2/3) T_e \)) from solution of Boltzmann' Equation for the electron energy distribution.
When electron energy deposition is non-collisional and/or transport is non-diffusional, Monte Carlo techniques are used.

- Secondary electron emission and acceleration through sheaths.
- Wave heating and trapping.
- Long mean-free-path transport.

Conduction currents are kinetically derived from the MCS for use in solving the wave equation.

\[ J_e(r) = J_0(r) \exp(i\phi_V(r)) \hat{\theta} = -q n_e(r) v_\theta(r) \exp(i\phi_V(r)) \hat{\theta}. \]
PLASMA CHEMISTRY, TRANSPORT AND ELECTROSTATICS

- Multi-fluid techniques are used where continuity, momentum and energy equations are solved for each species, with coupling terms for exchange of momentum and energy.

$$\frac{\partial N_i}{\partial t} = -\nabla \cdot (N_i \vec{v}_i) + S_i$$

$$\frac{\partial (N_i \vec{v}_i)}{\partial t} = \frac{1}{m_i} \nabla (kN_i T_i) - \nabla \cdot (N_i \vec{v}_i \vec{v}_i) + \frac{q_i N_i}{m_i} (\vec{E} + \vec{v}_i \times \vec{B}) - \nabla \cdot \vec{\mu}_i$$

$$- \sum_{j}^{m_j} \frac{m_j}{m_i + m_j} \frac{N_i N_j (\vec{v}_i - \vec{v}_j) \nu_{ij}}{\mu}$$

$$\frac{\partial (N_i e_i)}{\partial t} + \nabla \cdot Q_i + P_i \nabla \cdot U_i + \nabla \cdot (N_i U_i e_i) = \frac{N_i q_i^2 \vec{v}_i}{m_i (\vec{v}_i^2 + \omega^2)} E^2$$

$$+ \frac{N_i q_i^2}{m_i \vec{v}_i} E^2 S + \sum_{j}^{m_j} \frac{m_j}{m_i + m_j} N_i N_j R_{ij k} B(T_j - T_i) \pm \sum_{j}^{m_j} 3 N_i N_j R_{ij k} B T_j$$

- Slip boundary conditions are used for neutral transport for momentum and energy to address momentum and temperature jump conditions.
Given the hierarchy of time scales and large number of species, fully implicit solutions of all transport equations are typically not done.

Due to the extremely short dielectric relaxation times ($< 10^{-12}$ s), Poisson's equation must be implicitly solved.

A typical method uses a prediction of densities for the time at which the fields will be used. Surface charges are included here.

$$\nabla \cdot \varepsilon \nabla \Phi(t + \Delta t) = - \left( \rho_s + \sum_i q_i N_i - \Delta t \cdot \sum_i \left( q_i \nabla \cdot \vec{\phi}_i \right) \right)$$

When sheaths are not resolved by the mesh, semi-analytic models are used to obtain sheath potentials, which are inserted as potential "jump-conditions" at surfaces.
CIRCUIT MODELS

• Circuit models for the reactor and driving electronics provide voltage harmonics (amplitude and phase) on metal surfaces for solution of Poisson's equation.

• Sheath models are typically employed to account for non-linearities in the plasma response to harmonic excitation.
The MCFP model predicts time and spatially dependent etch profiles using neutral and ion fluxes from the PCMCS.

Any chemical mechanism may be implemented in the MCFP using a "plasma chemistry" input hierarchy.

\[ \text{Cl}^+ + \text{SiCl}_2(s) \rightarrow \text{SiCl}_2(g) \]

All pertinent processes can be included: thermal etch, ion assisted etch, sputter, redeposition, passivation.

Energy dependent etch processes may be implemented using parametric forms.

The MCFP may utilize ALL flux statistics from the PCMCS

- Ion energy and angular distributions
- Neutral energy and angular distributions
- Position dependent fluxes

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PROFILE CONTROL FOR INTERCONNECT: ETCH AND DEP

FLUOROCARBON ETCHING OF DIELECTRICS

IONIZED METAL PVD OF COPPER
Flotocarbon plasma etching of SiO$_2$ relies on a complex chemistry comprised of polymerization and chemically enhanced sputtering.

- Growth of C$_x$F$_y$ passivation layer (balance of deposition and consumption)
- Formation of a complex at the interface between oxide and passivation layer resulting from chemisorption of CF$_x$.
- Ion activated (through polymer layer) etching of complex in a two step process. Activation scales inversely with passivation layer thickness.
- Diffusion of etch precursor and etch product through layer.

![Diagram of plasma etching process]
The SKM was used to investigate the C$_2$F$_6$ etching of SiO$_2$ in an ICP reactor.

Representative gas phase chemistry:

- $e + C_2F_6 \rightarrow CF_3^+ + CF_3 + e + e$
- $e + C_2F_6 \rightarrow CF_3^- + CF_3$
- $e + CF_3 \rightarrow CF_2 + F + e$
- $e + CF_3 \rightarrow CF_2 + F^-$
- $e + CF_3 \rightarrow CF_3^+ + e + e$
- $e + CF_4 \rightarrow CF_2 + F + F + e$
- $F + F + M \rightarrow F_2 + M$
- $CF_2 + F_2 \rightarrow CF_3 + F$
- $CF_3 + F_2 \rightarrow CF_4 + F$
- $CF_3 + F \rightarrow CF_4$
- $CF_2 + F \rightarrow CF_3$

Electron Density

C$_2$F$_6$, 10 mTorr, 100 sccm, 650 W ICP, 100 V bias.
In SiO2 etching, passivation is a requirement and a hinderance.
- CF$_x$ is required as a precursor for removal of oxygen in the oxide.
- Passivation slows the delivery of activation energy to the surface.
- At low bias, the passivation decreases with increasing bias due to ion sputtering, etch rate increases due to higher activation power to surface.
- At high bias, the process is passivation starved and the etch rate saturates.

Solid:  $\Gamma_n / \Gamma_{ion} = 35$
Dashed: $\Gamma_n / \Gamma_{ion} = 25$

C$_2$F$_6$, 10 mTorr, 100 sccm, 650 W ICP
In high aspect ratio (AR) etching of SiO$_2$ by fluorocarbon plasmas, the sidewall of trenches are passivated by neutrals (CF$_x$, $x \leq 2$) due to the broad angular distributions of neutral fluxes.

Tapered trench profiles are produced when the passivation/ion flux ratio is large.

Experiment (C. Cui, AMAT)

Simulation

- Ar/C$_2$F$_6$ = 20/80.
- 1000 W ICP power, 150 V bias.
- 10 mTorr.
- Radial location: 3 cm.
PASSIVATION/ION FLUX RATIO

- Increasing passivating neutral to ion flux ratio ($\Gamma_n/\Gamma_{ion}$) leads to more tapered profiles due to increasing sidewall passivation.

- When the passivating neutral flux is too small, insufficient sidewall protection by the passivation layer leads to a bowed profile.
The bottom critical dimension of the trench decreases with increasing passivating neutral to ion flux ratio ($\Gamma_n/\Gamma_{ion}$).

The SiO$_2$ etch rate also decreases with increasing neutral flux due to increasing passivation.

$W_b$: Trench width 0.5 um above the bottom.

$W_t$: Trench width at the top.

Depth: Trench depth after equal etch time steps.
INFLUENCE OF ION ENERGY

- With increasing ion energy, the increasing ion sputtering yield of the sidewall passivation layer produces a less tapered profile.
- The etch rate also increases with increasing ion energy due to decreasing (but sufficient) passivation.
- Simulations and experiments obtained similar trends.

Experiments (C. Cui, AMAT)

<table>
<thead>
<tr>
<th>Bias Power</th>
<th>SiO$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>800 W</td>
<td></td>
</tr>
<tr>
<td>1000 W</td>
<td></td>
</tr>
</tbody>
</table>

Simulations

<table>
<thead>
<tr>
<th>Bias Voltage</th>
<th>SiO$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>150 V</td>
<td></td>
</tr>
<tr>
<td>180 V</td>
<td></td>
</tr>
</tbody>
</table>

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• When the ion energy is very high, the SiO$_2$ etching is limited by the ion flux instead of the ion sputtering yield.

• The etch rate and the bottom width of the trench are saturated at high ion energies.

![Graph showing $W_b/W_t$ vs Substrate Bias (V)]

- $W_b$: Trench width 0.5 um above the bottom.
- $W_t$: Trench width at the top.
- Depth: Trench depth after equal etch time steps.

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• Ionized Metal PVD (IMPVD) is being developed to fill deep vias and trenches for interconnect, and for deposition of seed layers and diffusion barriers.

• In IMPVD, a second plasma source is used to ionize a large fraction of the sputtered metal atoms prior to reaching the substrate.

**Typical Conditions:**

- 10’s mTorr Ar buffer
- 100s V bias on target
- 100s W - kW ICP
- 10s V substrate bias
In Physical Vapor Deposition (PVD), the majority of the metal flux to the substrate is neutral, having a broad angular distribution. This leads to nonconformal deposition and creation of voids.

In IMPVD, the addition of anisotropic metal ions to the flux produces conformal deposition by anisotropic filling and sputtering of overhangs.
PVD/IMPVD OF Cu: REACTOR LAYOUT

- PVD/IMPVD reactor with Cu Target
- 3.5-20 mTorr Ar (constant pressure), 150 sccm
- Annular magnetic field (200 G below target)
- Target: -200 V dc (2.4 kW)
- Substate: 40 V, 10 MHz, 350 W
- Coils: 2 MHz, 1250 W with Faraday shield

- Physics included:
  - Gas heating by sputtered target atoms
  - Ion energy dependent sputter yield
  - Neutral and ion momentum and energy
  - Bulk electron energy equation
  - Monte Carlo secondary electrons
  - Cross field Lorentz forces
The added inductively coupled electric field from the rf coils heats electrons in the bulk plasma producing a peak in temperature away from the target.

- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz
The combination of the magnetron fields and heating from the rf coils produces a more extended electron source and electron density. The ion density is 75% argon.

- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz
The magnetron focus the ion flux to the target, producing a sputter source of Cu atoms.

Due to the high gas pressure, the Cu atoms are thermalized in the vicinity of the target.

- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz
IMPVD TOOL: Cu DENSITIES

- Due to the longer residence time of Cu in the chamber and the higher electron temperature produced by the rf heating, the Cu inventory is largely converted to ions and metastables \([\text{Cu}^{(2D)}]\).

- \(\text{Cu}^{(2S)}\)
- \(\text{Cu}^{(2D)}\)
- \(\text{Cu}^+\)

- Ar, 20 mTorr
- -200 V Target, 200 G
- 1.25 kW ICP, 2 MHz
TRENCH FILLING VS PRESSURE

- *Operating conditions:
  - 1 kW ICP
  - 0.3 kW magnetron
  - -25 V dc bias on wafer

- Voids form at low pressure. The voids fill with increasing pressure and fill at 40 mTorr.

- The ionization fraction of increases with increasing pressure, due to slowing of Cu atoms which allows more ionization.

- Reasons for pinch-off:
  - Diffuse angular distribution of the neutrals
  - Less sputtering of over-hanging deposits

TRANSITION FROM PVD TO IMPVD

• With increasing ICP power deposition, a larger proportion of the Cu metal flux striking the substrate is ionized.

• The end result is conformal trench filling and elimination of the void.

• Ar 30 mTorr, 300 W Magnetron, -30 V bias
Further improvements in plasma equipment modeling will require improvements in both methods and availability of fundamental data.

<table>
<thead>
<tr>
<th>PHENOMENON</th>
<th>TOOL TYPE</th>
<th>EQUATIONS &amp; METHODS</th>
<th>STATUS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electromagnetics</td>
<td>ECR, ICP, HELICON, HFCCP</td>
<td>Maxwell Eqs.</td>
<td>Robust solvers available. Time domain is difficult.</td>
</tr>
<tr>
<td>Magnetostatics</td>
<td>MERIE, PVD, HELICON</td>
<td>Maxwell Eqs.</td>
<td>Robust solvers available.</td>
</tr>
<tr>
<td>Electrostatics</td>
<td>ALL</td>
<td>Poisson’s Eq.</td>
<td>Better implicit solvers are needed. Very high bias, magnetic fields difficult.</td>
</tr>
<tr>
<td>Electron Energy Transport</td>
<td>ALL</td>
<td>Monte Carlo, Fluid Eqs.</td>
<td>Robust solvers which are computationally efficient are required. High magnetic fields difficult.</td>
</tr>
</tbody>
</table>
# IMPORTANT PHYSICS, METHODS, STATUS

<table>
<thead>
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<th>EQUATIONS &amp; METHODS</th>
<th>STATUS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutral and Ion Transport</td>
<td>ALL</td>
<td>Compressible, multi-fluid Navier Stokes</td>
<td>Robust solvers available. High magnetic fields difficult. Long term transients difficult.</td>
</tr>
<tr>
<td>Sheath Physics</td>
<td>ALL</td>
<td>Semi-analytic models</td>
<td>Physics understood but difficult to implement for &quot;harsh&quot; conditions.</td>
</tr>
<tr>
<td>Long Mean Free Path Transport</td>
<td>PVD, ECR</td>
<td>Monte Carlo, Greens Function</td>
<td>Robust methods which take large CPU time.</td>
</tr>
<tr>
<td>Surface Chemistry</td>
<td>ALL</td>
<td>Multi-layer surface site-balance</td>
<td>Robust solvers available. Limited by availability of fundamental data.</td>
</tr>
<tr>
<td>Profile Evolutions</td>
<td>ALL</td>
<td>Monte Carlo, Level set, String methods</td>
<td>Robust solvers available. Charging models uncertain. Limited by availability of fundamental data.</td>
</tr>
</tbody>
</table>
• Plasma equipment modeling has developed to the point that quantitative design of tools can be performed and the design cycle can be shortened.

• Process design based on modeling is in a more qualitative state, though progress is being made.

• Significant improvements are required in our databases of fundamental parameters (e.g., cross sections) so that more complex plasma chemistries can be addressed.
For a copy of today's presentation......

http://uigelz.ece.uiuc.edu → Presentation link at top of page