SPUTTER-WIND HEATING IN IONIZED METAL PVD+

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AGENDA

• Introduction to IMPVD
• Overview of Hybrid Plasma Equipment Model
• Description of sputter model
• Validation of sputter model
• Results and discussions for Al IMPVD
  • Investigating the effects of sputter heating by comparing to the results without sputter heating
    • Plasma properties
    • Depositing Al fluxes
  • Ar and electron densities as functions of magnetron and ICP power
• Summary
IONSIZED METAL PHYSICAL VAPOR DEPOSITION (IMPVD)

- 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:
  - 10-30 mTorr
  - Ar buffer
  - 100s V bias on target
  - 100s W - a few kW ICP
  - 10s V bias on substrate
Ions are able to fill deep trenches because their spread in angles is narrowed by the rf bias.
SPUTTER GAS HEATING IN IMPVD

- In IMPVD processes, two types of atoms produced in the sputtering process transfer momentum and energy to background gas atoms, (sputter heating)
  - Sputtered metal atoms
  - Reflected neutral atoms produced by the incident ions
- The degree of sputter heating increases with:
  - Magnetron power
  - Sputter yield
  - Collision cross section of the gas
- This sputter heating affects
  - Background gas density
  - Ion flux to the target
  - Sputtered atom flux and the depositing metal flux
- To investigate the effects of sputter heating, we incorporated a sputter algorithm into a Hybrid Plasma Equipment Model (HPEM).
SCHEMATIC OF 2-D/3-D HYBRID PLASMA EQUIPMENT MODEL

- **PLASMA CHEMISTRY MONTE CARLO SIMULATION**: 
  - $E_S(r,z)$, $V(r,z)$
  - $S(r,z)$

- **ETCH PROFILE MODULE**: 
  - FLUXES

- **MAGNETOSTATICS MODULE**: 
  - $B(r,z)$
  - $E_\Theta(r,z,\phi)$, $B(r,z,\phi)$

- **CIRCUIT MODULE**: 
  - $I,V$ (coils)
  - $E_\Theta(r,z,\phi)$

- **ELECTROMAGNETICS MODULE**: 
  - $E_\Theta(r,z,\phi)$, $E_\phi(r,z,\phi)$

- **FDTD MICROWAVE MODULE**: 
  - $\sigma(r,z)$, $I$ (coils), $J(r,z,\phi)$

- **ELECTRON MONTE CARLO SIMULATION**: 
  - $E_\Theta(r,z,\phi)$

- **ELECTRON BEAM MODULE**: 
  - $E_\Theta(r,z,\phi)$

- **ELECTRON ENERGY EQN./BOLTZMANN MODULE**: 
  - $E_\Theta(r,z,\phi)$

- **NON-COLLISIONAL HEATING**: 
  - $S(r,z)$, $T_\Theta(r,z)$

- **FLUID-KINETICS SIMULATION**: 
  - $\Phi(r,z,\phi)$

- **HYDRODYNAMICS MODULE**: 
  - $V(rf), V(dc)$

- **ENERGY EQUATIONS**: 
  - $\Phi(r,z,\phi)$

- **SHEATH MODULE**: 
  - $R$

- **LONG MEAN FREE PATH (SPUTTER)**: 
  - $R$

- **SIMPLE CIRCUIT**: 
  - $\Phi(r,z,\phi)$

- **EXTERNAL CIRCUIT MODULE**: 
  - $\Phi(r,z,\phi)$

- **MESO-SCALE MODULE**: 
  - $R$

- **SURFACE CHEMISTRY MODULE**: 
  - $R$

- **VPEM: SENSORS, CONTROLLER, ACTUATORS**: 
  - $E_S(r,z,\phi)$

- **ELECTRON BEAM MODULE**
  - $E_\Theta(r,z,\phi)$

- **ELECTRON MONTE CARLO SIMULATION**
  - $E_\Theta(r,z,\phi)$

- **FLUID-KINETICS SIMULATION**
  - $\Phi(r,z,\phi)$

- **HYDRODYNAMICS MODULE**
  - $V(rf), V(dc)$

- **SIMPLE CIRCUIT**
  - $\Phi(r,z,\phi)$

- **EXTERNAL CIRCUIT MODULE**
  - $\Phi(r,z,\phi)$

- **MESO-SCALE MODULE**
  - $R$

- **SURFACE CHEMISTRY MODULE**
  - $R$

- **VPEM: SENSORS, CONTROLLER, ACTUATORS**
  - $E_S(r,z,\phi)$

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**OPTICAL AND DISCHARGE PHYSICS**

AVS99_05 HPEM
IMPROVEMENT TO SPUTTER ALGORITHMS

- To better model the IMPVD process, the following improvements have been made to the sputter algorithms in the HPEM
  - Ion energy-dependent yield for sputtered atoms
  - Ion energy-dependent kinetic energy for sputtered and reflected atoms
  - Momentum and energy transfer from sputtered and reflected atoms to the background gas atoms

- The energy-dependent yield of the sputtered atoms is

\[
Y(E_i) = \begin{cases} 
0.42 \frac{\alpha Q K_s n(\varepsilon)}{U_s (1 + 0.3 U_s s_e(\varepsilon))} \left(1 - \sqrt{E_{th}/E_i}\right)^{2.8}, & E_i > E_{th} \\
0, & E_i \leq E_{th}
\end{cases}
\]

*Masunami et al., At. Data Nucl. Data Tables 31, 1 (1984).*

- The effective yield of the reflected neutrals
  - 0.9 for high kinetic energy
  - 0.1 for thermal energy

![Graph showing yield of Ar⁺-Al pair vs. incident Ar⁺ energy (eV)]
ENERGY DISTRIBUTIONS
OF THE SPUTTERED AND THE REFLECTED ATOMS

- Energy of the emitted atoms obeys a cascade distribution:
  (Thompson’s law for $E_i \approx 100$’s eV):

$$ F(E) = \begin{cases} 
2 \left(1 + \frac{U_s}{\Lambda E_i}\right)^2 \frac{U_s E}{(U_s + E)^3}, & E \leq \Lambda E_i \\
0, & E > \Lambda E_i 
\end{cases} $$

- Reflected neutral energies are obtained from TRIM* and MD simulations.

**Ar+** incident on Al, David Ruzic, Depart. of Nuclear Engineering, UIUC.

- Kinetic energies of reflected neutrals are curve fitted into thermal accommodation coefficient ($\alpha$) vs. incident ion energy.

$$ \alpha = \frac{E_i - E_r}{E_i - E_T} $$

- For Ar+ incident on Al target, $\alpha \approx 0.95$. 

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AVS_07 ENERGY
The sputter model employs a kinetic Monte Carlo approach:

- **Sputter rate** = \( \text{Yield} \cdot (\text{ion flux} + \text{fast neutral flux}) \)

- Sputtered atoms and reflected neutrals are emitted with a cosine distribution in angle.

- Collisions of sputtered atoms and reflected neutrals with the background gas are assumed to be elastic.
OVERVIEW OF SPUTTER MODEL (Continued)

• Recording of sputtered metal atoms and reflected neutrals
  • Thermalized → Green’s Function
  • In-flight → local density

• Incorporation of statistics into fluid equations

- Rate of Change of Momenta and Energy
- Thermalized Atoms

- Source Terms

- Fluid Equations

• Quantities of interest generated
  • Metal atom densities in the plasma
  • Metal flux to the wafer
  • Gas heating terms
MODEL VALIDATION: Al IMPVD

• HPEM IMPVD model was validated by comparing with experiment (Dickson and Hopwood, J. Vac. Sci. Technol. A 15(4), 1997, p. 2307)

• Good agreement with experimental data:
  • V-I characteristic
    | Voltage (V) | HPEM | EXP. |
    | Current (A) | 255  | 240  |
    | 0.94        |      | 1.0  |

• Ionization fraction of Al at r = 4 cm
  | Distance (cm) | HPEM | EXPERIMENT |
  | 10 (plasma)   | 15%  | 10-15%     |
  | 12 (flux)     | 73%  | 70%        |

• Predicted and measured Al densities = $10^{11}$ cm$^{-3}$ at r = 4 cm, 8-10 cm below target.
SPUTTER HEATING: Ar DENSITY

- Modified TEL IMPVD tool.

- Operating conditions
  - 0.5 kW ICP
  - 1.0 kW magnetron
  - 30 V rf on substrate
  - 30 mTorr Ar

- The minimum Ar density
  - Decreases by 30% with sputter heating
  - Occurs below target due to sputter heating and charge exchange

- Contribution to sputter heating
  - Reflected neutrals 2/3.
  - Sputtered metals atoms 1/3.
• Exponential decay of the magnetic field away from the magnets.

• Peaks of Ar\(^+\) fluxes due to the magnetic cups.

• Sputter heating increases the Ar\(^+\) density near the center of reactor.

• The target voltage is -178 V with sputter heating, and -168 V without.

• Decreasing Ar\(^+\) density below target leads to a lower ion current and a higher voltage for the same magnetron power.
• $T_e(\text{max})$ below the target is caused by energetic secondary electrons and joule heating.

• $T_e$ decreases by 1 eV with sputter heating. This agrees with observations (Dickson, Qian, and Hopwood, JVST A 15 (2), 340 (1997)).

• The electron temperature is high near the coils, due to inductive heating.
SPUTTER HEATING: AI DENSITY

- The maximum Al density with sputter heating is only 1/3 of that without, due to the longer mean free path.

- Since the magnetron power is the same, the amount of sputtered Al atoms is about equal in both cases.

- Sputter heating redistributes Al in the reactor to conserve the total inventory of Al atoms.

- The Al density with sputter heating decays much slower from the target to the substrate.
SPUTTER HEATING: Al\(^+\) DENSITY

- The Al\(^+\) density with sputter heating has a broader peak and decreases slower toward the substrate, due to the longer mean free path in a more rarefied gas.

- Note the depletion of Al\(^+\) ions by the target bias with sputter heating.
• The total depositing metal flux consists mostly of Al\(^{+}\) and thermal Al atoms.

• The direct Al flux is negligible because of long throw distance (15 cm, \(~10\) mfp), and Al\(^{+}\) is depleted by ionization.

• The magnitude of the Al flux with sputter heating is \(>2\) times that without, while the ionization fraction decreases to 67-86% from above 90%.
Both the minimum and the reactor averaged Ar densities decrease with increasing magnetron power due to increasing sputter heating.

The minimum Ar densities converge at high magnetron power:
- The specific power density decreases due to longer stopping distance.
- The minimum gas density occurs right below the target, and the heat loss to the target increases as the gas temperature increases.
The electron density significantly increases when magnetron power is increased from zero due to low-ionization potential metal atoms.

As the magnetron power further increases, the electron density saturates due to decreasing Al ionization fraction.

At constant magnetron power, electron density increases linearly with ICP power.

- Average electron density
SUMMARY OF SPUTTER HEATING STUDY

• Sputter heating from both sputtered metal atoms and reflected neutrals significantly rarefies the background gas, thus increasing the mean free path for transport of the sputtered atoms and redistributing metal species in the reactor.

• Sputter heating decreases the ionization fraction of the depositing metal flux, but increases its magnitude, similar to operating at lower pressure.

• Sputter heating should NOT be neglected in the modeling of IMPVD processes.

• The addition of small amount of metal atoms with low ionization potential significantly increases the electron density.

• Electron density tends to saturate with increasing magnetron power since gas rarefaction reduces the ionization fraction of the metal atoms.