AN INTEGRATED PLASMA EQUIPMENT-FEATURE SCALE MODEL FOR IONIZED METAL PHYSICAL VAPOR DEPOSITION⁺

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AGENDA

- Introduction to IMPVD
- Description of the model and the sputter algorithm
- Metal densities, electron temperature and density in Cu IMPVD
- Diffusion model for profile simulation
- Trench filling at different pressures, magnetron and ICP power
- Conclusions

IONIZED 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 the sputtered metal atoms prior to reaching the substrate.



• lons are able to fill deep trenches because their angular distributions are narrowed by the rf bias.



COMPUTATIONAL PLATFORM



- Ion energy-dependent yield* for sputtered atoms.
- The effective yield of 1 for the reflected neutrals.
- Ion energy-dependent kinetic energy
 - Sputtered atoms: Cascade distribution
 - Reflected neutrals: TRIM** and MD***
- Cosine distribution in angle for sputtered and reflected atoms emitted from target.
- Momentum and energy transfer from sputtered and reflected atoms to background gas (sputter heating).
- Electron impact ionization for in-flight sputtered and reflected neutrals.
- Source terms for thermalized sputter species and gas heating.

*Masunami et al., At. Data Nucl. Data Tables 31, 1 (1984) . **D. Ruzic, UIUC. ***Kress et al., J. Vac. Sci. Technol. A 17, 2819 (1999)



- Reactor is based on *Cheng et al.
- Operating conditions:
 - 40 mTorr Ar
 - 1.0 kW ICP
 - 0.3 kW magnetron
 - -25 V dc bias on substrate
- Cu peaks below the target since most of the sputtered Cu atoms are thermalized a few cm below the target.
- Cu⁺ peaks at the center due to the depletion of ions by the biased target and the substrate.

*Cheng, Rossnagel, and Ruzic, JVST 13(2), 1995, p. 203.



Cu IMPVD: ELECTRON TEMPERATURE AND DENSITY

- The electron temperature is > 3 eV throughout the reactor.
- The large T_e near the coils is due to the large ICP power deposition in this region.
- The electron density peaks off center due to the magnetron effect and off-axis ionization by ICP power.



MONTE CARLO FEATURE PROFILE MODEL (MCFPM)



- The MCFPM obtains the etch and deposition profile using ion and neutral distributions from the PCMCS.
- Surface processes are implemented using a chemical reaction mechanism:
 - Deposition: Cu(g) + Si(s) --> Cu(s) + Si(s)
 - Resputtering: $Ar^+(g) + Cu(s) \rightarrow Ar(g) + Cu(g)$
- The model takes account of angular and energy dependent etch and deposition rates.
- The model could simulate many different chemistries and material mesh.

• E_A

• T

SURFACE DIFFUSION ALGORITHM IN MCFPM

- To reduce unphysical dendritic growth obtained during IMPVD, a diffusion algorithm was incorporated into the MCFPM.
- Diffusion probability (P_{DIF}) of the surface "cell" is*

$$P_{DIF} = \exp(-E_A / k_B T), \qquad E_A = E_{NEW} - E_{OLD}$$

- activation energy for diffusion surface temperature sum of potential (V) at locations • E_{NEW}, E_{OLD} before and after diffusion
- The potential (V) between two cells is given by a mesh-modified Morse potential.
- For Cell 0 to diffuse to location 5, the contributing cells to potential are:
 - Cells 1, 2, 3, 4 for E_{OLD} of Cell 0
 - Cells 4, 9, 10, 11 12, 13 for E_{NEW} of Cell 5

*W. Helin et al., Vacuum 52, 435-440 (1999).





TRENCH FILLING WITH AND WITHOUT DIFFUSION

- Without diffusion, the Cu films are unphysically porous and non-conformal.
- With diffusion, Cu species deposit compactly and conformally.
- The majority of Cu⁺ are incident at 55 eV, and within 12 degrees of the normal.

Trench Aspect Ratio = 1.1, Trench Width = 600 nm Cu⁺ : Cu Neutrals = 4:1





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

*Cheng, Rossnagel and Ruzic, JVST B 13, 203 (1995).





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TRENCH FILLING WITH AND WITHOUT RESPUTTERING

Ar+: Cu Total = 7:1 Cu+: Cu Neutrals = 4:1

1.2 **No Resputtering** With Resputtering Height (μm) 0.8 0.4 0 1.2 Height (μm) 0.8 0.4 0 0.4 0.8 1.2 0.4 0 0.8 1.2 0 Width (µm) Width (µm)

- Without resputtering, the overhang deposits grow faster than the bottom deposits, and this leads to pinch-off at the top.
- Resputtering reduces the overhang deposits, opens up the top of the trench, and enables more fluxes to arrive at the bottom.
- Note that Ar⁺ contributes significantly to resputtering.

TRENCH FILLING VS MAGNETRON POWER

- Operating conditions: 30 mTorr Ar, 1 kW ICP, -30 V dc bias on wafer.
- As magnetron power increases, the incident ion flux and the target bias increase, and more Cu atoms are sputtered into the plasma.
- The ionization fraction of the Cu atoms decreases since more power is required maintain the same ionization fraction.
- The small void at low magnetron power was caused by microtrenching.



TRENCH FILLING VS ICP POWER

- Operating conditions: 30 mTorr Ar, 0.3 kW magnetron, -30 V dc bias on wafer.
- As ICP power decreases, the power available for Cu ionization decreases, and the Cu ionization fraction decreases.
- The pinch-off at low ICP power is caused by low ionization fraction.



CONCLUDING REMARKS

- An integrated plasma equipment-feature scale model has been developed and applied to IMPVD modeling.
- Surface diffusion is an important process in metal deposition.
- The deposition model was validated by comparing to experimental observations.
- Formation of voids in trench filling occurs when the ionization fraction of the depositing metal flux is low.
- Both the directionality of ions and resputtering of overhang deposits are beneficial to trench filling.
- The desirable conditions for complete trench filling are high pressure, low magnetron power, and high ICP power.