Global modeling of HiPIMS systems: transition from homogeneous to self organized discharges

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High Power Pulse Magnetron Sputtering

- Ionized Physical Vapor Deposition technique
- High degree of ionization of sputtered vapor allows film growth control and high film quality
- High power pulse of low frequency and low duty cycle to cathode

Characteristics of HiPIMS plasmas: Film quality vs. efficiency

- **PRO**: Highly energetic metal ions (≈ 10 eV)
- **CONTRA**: Reduced deposition rate (µm/h)

- HiPIMS plasmas are non-stationary and show self-organization in symmetry breaking structures
- Plasma composition evolves during discharge

A Hecimovic, et al., PSST, 21 (2012) 35017
Plasma regimes: different self-organization and chemistry

- Regime II: emission 'chaotic'
- Regime III: stable rotating frequency: spokes
- Regime IV: homogeneous emission

Winter, J Phys D 46, 84007 (2013)

de los Arcos, J Phys D 46, 335201 (2013)
Working Hypothesis on Spokes Formation and Evolution

- HiPIMS discharges sustained by secondary electrons (metal target at -500 V)
- Only Ar\(^+\) and M\(^{2+}\) produce secondary electrons, M\(^+\) cannot (density M\(^+\) \gg M^{2+}\))
- Intermediate/high currents \(\rightarrow\) high sputtering \(\rightarrow\) high metal density \(\rightarrow\) self sputtering

![Diagram showing sputtering, self sputtering, and quenching]

- High M and M\(^+\) density \(\rightarrow\) discharge quenches
- Discharge re-organizes into "spokes", which rotate toward regions of low M and high Ar density
- High ionization regions (spokes) not necessary once population of M\(^{2+}\) sufficiently high.
Homogeneous Volume-Averaged Models

Rate equations for heavy species:

\[ n_{\text{Ar}}, \; n_{\text{Ar}^+}, \; n_{\text{Ar}^*-4s}, \; n_{\text{Ar}^*-4s'} \]
\[ n_{\text{Al}}, \; n_{\text{Al}^+}, \; n_{\text{Al}^{2+}} \]

Integrated collision cross sections \( \sigma_j \) (m\(^2\))

Maxwellian Equilibrium Global Model (MEGM):

Electron continuity and energy conservation equations

- Low current

Kinetic Global Model (KGM):

Boltzmann’s equation for an isotropic eedf \( f(\varepsilon, t) \)

- Low current
- Intermediate current
- High current
Convergence Procedure

Raw experimental data

Iteration until calculated matches imposed current

MEGM: $P \propto \eta_{PWR} \frac{I_D V_b}{e V_{IR}}$

KGM: $S(\varepsilon, t) = \eta_{PWR} \gamma_{sec} \frac{I_{Ar}(t)}{e V_{IR}} G(\varepsilon)$

Convergence Procedure: eventual feedback

Variable resistance modeled via time varying power coupling efficiency

Raw experimental data

Iteration until calculated matches imposed current

On the fly feedback for better convergence

\[ V_b \]
\[ R_c \]
\[ \eta_{PWR} \]
Low current case ($2 \cdot 10^2 \text{ mA/cm}^2$)

Already at low current, the MEGM is inappropriate

dashed: MEGM
solid: KGM
**Intermediate current case (1 \cdot 10^3 \text{ mA/cm}^2)**

doubly charged ions non relevant

need feedback on coupling efficiency
High current case (4 \cdot 10^3 \text{ mA/cm}^2)

Al^+ cannot produce secondary electrons
Al^{2+} still negligible

onset of self sputtering
Compare all current cases

For all cases: ion species drift to target as soon as created

\[ k_{\text{Al,ion}} n_e n_{\text{Al}} = \Gamma_{\text{Al}} \frac{S_{\text{RT}}}{V_{\text{IR}}}, \quad k_{\text{Ar,ion}} n_e n_{\text{Ar}} = \Gamma_{\text{Ar}} \frac{S_{\text{RT}}}{V_{\text{IR}}} \]

Differences come into play in Al rate eqn

\[ \frac{dn_{\text{Al}}}{dt} \approx -k_{\text{Al,ion}} n_e n_{\text{Al}} - \frac{\Gamma_{\text{Al,diff}}}{L} + \left( \Gamma_{\text{Al,Yssp}} + \Gamma_{\text{Al,Ysp}} \right) \frac{S_{\text{RT}}}{V_{\text{IR}}} \approx -\frac{\Gamma_{\text{Al,diff}}}{L} + k_{\text{Ar,ion}} n_e n_{\text{Ar}} \]

\[ \begin{cases} \leq 0 - \text{low to intermediate } I_D \\ > 0 - \text{high } I_D \end{cases} \]

need to enhance Al diffusion and Ar ionization!

\[ \times 5 \text{ Al diff} \]
\[ \times 10 \text{ Ar diff} \]
Conclusions

- High M and M$^+$ density $\rightarrow$ discharge quenches ✓
- Discharge re-organizes into "spokes", which rotate toward regions of low M and high Ar density ✓
- High ionization regions (spokes) not necessary once population of M$^{2+}$ sufficiently high $\rightarrow$ WIP

if enough Ar is ionized the discharge can be maintained even in self sputtering $\rightarrow$ moving ionization regions
Thank you for the attention

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