Modélisation particulaire du plasma magnétron impulsionnel haute puissance

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Plasma deposition process

Gas dynamics

Film growth

Particle transport

Sputtering

D Lundin et al., P S S T 18, 045008 (2009)
Conventional magnetron discharge

- **Metal** sputtering wind from the target
- **Energetic Ar** backscattering
- **Temperature increases**

Local **gas rarefaction** in the high and dense plasma region due to the “wind” effect

**High Power Impulse Magnetron Sputtering**

**HiPIMS**

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**First Pulsed generator concept**

V. Kouznetsov, U. S. Patent No. 6,296,742 B1 (2001)

- **Pulsed power supply:**
  - 0.1 – 1 kHz, 200 A, 1 kV
- **Pulse width:** 50 to 200 µs
- **Average pulse power:** 50 kW
- **Typical mean power:** 500 W

**SINEX 3 power supply by PlasmAdvance**

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T. Minea  
Outline

1. Dimensional modelling of HiPIMS magnetron plasma (OHIPIC)

2. 2D Charged Species and Sheath evolution

3. \textit{a posteriori} Monte Carlo

4. Metal Transport (3D I-OMEGA)

5. ‘Spokes’ Modelling – ITC LPGP-ICARE

6. Conclusions
Debye length

\[ n_e = 10^{13} \text{ cm}^{-3} = 10^{19} \text{ m}^{-3} \]
\[ \lambda_e \approx 10 \mu\text{m} \ (T_e = 4\text{eV}) \]

Geometry \((x, z)\)

- Simulation volume: 2 \(\times\) 2.5 cm\(^2\)
- Grids: 201 \(\times\) 512 \(\div\) 401 \(\times\) 2048
- Cell dimensions: \(\Delta x, \Delta z = 10 \mu\text{m} \) !!!
- 6 million simulation particles

Control parameters

- Time step: \(\Delta t = 5 \times 10^{-12} \text{ s} \div 5 \times 10^{-13} \text{ s} \)
- Simulated real time: 3.5 \(\mu\text{s} \) !!!
Numerical stability criteria

Stability criteria:

- $a < \lambda_{De}$
- $\text{CFL} : v_e \times \Delta t < a$
  (Courant, Friedrichs, Lewy)
- $N^\circ \text{particle/cell} \sim 50$

*Fluctuation of the net charge density (Rho)*

Adrien REVEL & Tiberiu MINEA
HiPIMS Simulation parameters

**Plasma \((e, Ar^+)\) parameters:**
- \(Ar\) gas + Cu target
- \(p = 5\) mtorr
- \(T_{Ar} = 400\) K

**Magnetic field structure**

**Short pulse**

**Pre-ionization**

\[ \begin{array}{c}
A (75\, \text{ns}) \\
B (2\, \mu\text{s}) \\
C (3\, \mu\text{s})
\end{array} \]
Fast HiPIMS with pre-ionization

**SHORT & FAST** Pulsed Power Supply concept [*] which uses
- **pre-ionization** to guarantee the **fast rise time** of the current,
- **fast fall time** of the discharge voltage at the switch-off

- **Average Power** 80 W
- **Pulse width**: \( \sim 10 \, \mu s \)
- **Repetition rate**: 50-500 Hz
- \( U_{\text{max}} \sim 1 \text{kV} \)
- \( I_{\text{Max}} : 10-100 \, \text{A} \)

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* Ganciu et al,
HiPIMS current

**OHIPIC: Orsay HIgh density plasma Particle-In-Cell model**

**Experiment**

**OHIPIC simulated discharge current**

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2D maps of charged particles by OHIPIC

A (75 ns); \( n_e = 8 \times 10^{16} \text{ m}^{-3} \)

B (2 \( \mu \text{s} \)); \( n_e = 8 \times 10^{17} \text{ m}^{-3} \)

C (3 \( \mu \text{s} \)); \( n_e = 5 \times 10^{18} \text{ m}^{-3} \)

- Electron density increases \( \times 100 \) in 3 \( \mu \text{s} \) !!!
- Much localized high density
- Larger dense plasma=> larger race-track

To take home!
Axial profile evolution of charged particles by OHIPIC

- Highest local density = 2 x \( n_e \) in Ionization Region (IR)
- \( n_e \) in IR = 10 x \( n_e \) in Diffusion Region (DR)
Plasma potential evolution by OHIPIC

- Very high electric field in the sheath
- Constant but twice higher field in IR in HiPIMS compared to DC
- Very low field in DR
**eedf evolution in HiPIMS by OHIPIC**

- **2D HiPIMS modelling**
- **a posteriori MC**
- **3D Metal modelling**
- **Spokes Modelling**

### Graphs

**Graph 1:**
- EEDF (eV\(^{-3}\)) vs. Energy (eV)
- Curves for different time points: 75 ns, 0.5 μs, 1.0 μs, 1.5 μs, 2.0 μs, 2.5 μs, 3.0 μs

**Graph 2:**
- eepf (eV\(^{-3/2}\)) vs. Energy (eV)
- Curves for different volume regions: Total volume, z < 7.5 mm, z > 7.5 mm

**Graph 3:**
- EEDF (eV\(^{-1}\)) vs. Energy (eV)
- Data points at different distances: 0 μm, 2 μm, 4 μm, 7 μm, 10 μm, 15 μm, 20 μm, 25 μm, 30 μm

**Graph 4:**
- eepf (eV\(^{-3/2}\)) vs. Energy (eV)
- Curves for different volume regions: Total volume, z < 7.5 mm, z > 7.5 mm

*P Poolcharuansin and J W Bradley, PSST (2010)*
1. Dimensional modelling of HiPIMS magnetron plasma (OHIPIC)

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3. *a posteriori* Monte Carlo

4. Metal Transport (3D I-OMEGA)

5. ‘Spokes’ Modelling

6. Conclusions
- Critical point of Monte Carlo simulations
  - prior knowledge (‘guess!!!’) of the force field (interaction potential)
- Self-consistent 2D maps of plasma parameters by OHIPIC simulation
- Initial condition for test particles
Electron transverse diffusion in HiPIMS

On the pulse voltage plateau

**Drift velocity**

\[ w_x = \frac{d}{dx} \langle x \rangle \]

**Transverse Diffusion**

\[ D_{zz} = \frac{1}{2} \frac{d}{dt} \left\langle \left( z - \langle z \rangle \right)^2 \right\rangle \]

Electron deconfinement in HiPIMS??

C. Costin, T. Minea, G. Popa, P S S T (submitted)
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OMEGA: Orsay MEtal transport in GAses model

1. Define a domain (sputter chamber)
2. Generate sputtered particles one by one randomly from a probability distribution (SED + SAD)
3. DCMS: Particle collision with process gas
4. Analyze the particle’s velocity, direction, ...

OMEGA Results & Benchmarking DC

2D LIF measurements of Ti sputtered vdf


Assumptions I-OMEGA

- 3D treatment of elastic collisions as in OMEGA
- No Ti-Ti collisions, since $n_{Ti}/n_{Ar} < 0.2$
- No gas rarefaction

Inelastic electron impact ionization\(^1,2\)
External input of $n_e$ and $T_e$ maps

For IPVD we have to include ionization of sputtered particles
Inelastic collisions: $Ti + e \rightarrow Ti^+ + 2e$
Need cross sections\(^1,2\) + $n_e$ & $T_e$ 2D maps from OHIPIC
I-OMEGA still tracks neutral Ti
Ionization acts as a loss term for neutrals

How do we test the accuracy of I-OMEGA?

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HiPIMS means high plasma density ($\sim 1 \times 10^{19} \text{ m}^{-3}$) vs DC, $\sim 1 \times 10^{16} \text{ m}^{-3}$

- Increased probability for ionizing collisions, $\lambda_{\text{HiPIMS}} \sim 0.01 \text{ m}$ and $\lambda_{\text{DCMS}} \sim 0.50 \text{ m}$

**HiPIMS:** D. Lundin and K. Sarakinos, J. Mater. Res. 27, 780 (2012)

HiPIMS simulated by OHIPIC code

Density maps for the three representative instants of the pulse

- Short pulse Pre-ionization
  - A (75 ns)
  - B (2 µs)
  - C (3 µs)

- *a posteriori* MC very useful and powerful
- Fast estimation of the ionization fraction of sputtered vapour and metal ion back-attraction

To take home!
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Electron burst vs Spokes – top view


Electron burst – side view

\[ a \text{ posteriori} \quad \text{MC} \]

\[ \begin{array}{c}
\text{PRELIMINARY} \\
\end{array} \]

\[ \begin{array}{c}
\text{C. Costin \& T. Minea} \\
\end{array} \]

\[ \begin{array}{c}
\text{Fast camera} \quad \text{Anders, Ni, and Rauch} \\
\text{J. Appl. Phys. 111, 053304 (2012)} \\
\end{array} \]
Pseudo-3D PIC: Azimuthal PIC MCC

$2D \ (x,z) \ \text{PIC-MCC}$

$\Rightarrow \ E_x(x, z) \ & E_z(x, z)$

Pseudo 3D code calculation

$E_y(x, y, z) = \frac{1}{2} \cdot (E_{y, \text{red plane}}(x, y) + E_{y, \text{yellow plane}}(y, z))$

$2D \ (x,z) \ PIC-MCC$ with frozen $(x,z)$ field map

A. Revel, C. Costin, T. Minea (in preparation)
Case 1: Secondary electrons released mainly from the race-track ($\gamma = 0.1$)

Case 2: Secondary electrons localized over-emission by 10%

Spokes formation !!!
Side view of spokes flares

**PIC-MCC**

- y (mm)
- z (mm)
- Net charge density
- silt position

A. Revel, C. Costin, T. Minea (in preparation)

**Fast camera** Anders, Ni, and Rauch
Pseudo-3D PIC : time average density

Electron density integrated over 1 µs

NO spokes signature at µs time-scale!

Anders, Ni, and Rauch
Spokes origin

- **Anders et al.** - ion impact on the target (dependency with the gas mass and target sublimation energy)

- **Brenning et al.** - critical ionization velocity (CIV) when plasma moves with respect to background gas

\[ v_s = \sqrt{\frac{2eU_i}{M_i}} \]

- **Pflug et al.** – plasma instabilities

- **Costin & Minea** - Burst of electron released from the cathode surface, close to the race-track
Conclusions

- Particle simulations bring microscopic information in space and time on plasmas species (densities, potential, eedf, etc.)

- This knowledge of plasma can be exploited further to deduce transport parameter (electron diffusion across the magnetic field), instabilities, metal transport and ionization, kinetic channels, etc.

- Reactivity in HiPIMS is only initiated in the high power pulse phase, but it continues in the afterglow, by different reaction channels, namely negative ions
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