Studying Target Erosion in Planar Sputtering Magnetrons Using a Discrete Model for Energetic Electrons

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INTRODUCTION

PLANSEE SE

- founded in 1921 for production of molybdenum (Mo) and tungsten (W) wires
- annual turnover: € 1,500 M+ • employees: 6,000+ worldwide (2012)
- world market leader in P/M production of refractory metals

used in wide range of high-tech applications and industries: lighting, medical, power generation, aerospace ...

unique combination of material properties:
- high melting point
- excellent high temperature strength
Sputtering process

- PVD (physical vapor deposition) process
- for thin film deposition
- on various substrates
- source material (e.g. Mo and W)
- sputtered from “targets” by ion bombardment
- established by gas discharge

PLANSEE’s twofold role in sputtering

- supplier of targets made from Mo and W
- user of sputtering process for in-house coating
The magnetron sputtering process

- operated in vacuum chamber (typical pressure: $10^{-1} - 10^0$ Pa)
- target bonded onto cathode
- geometric layouts depending on field of application
- DC discharge:
  - stationary electric field between grounded anode and cathode subjected to negative bias (typically: -200 to -400 V)
  - formation of plasma with cathode fall (plasma sheath)
  - using background gas, e.g. argon (Ar)
- magnetically enhanced: static magnetic field providing “confinement” to electrons
INTRODUCTION

Magnetic confinement of energetic electrons

advantages:
- increased ionization and sputtering rate
  → allows reducing operating pressure
  → reduced spurious depositions
  → higher deposition quality

drawbacks:
- non-uniform ion flux onto target
  → non-uniform target erosion
  → reduced target utilization (typically: ~ 20 – 40 %)
- rectangular targets: cross corner effect (CCE)

Objective
- improve uniformity of target erosion
- increase target utilization
- by means of numerical simulation
  → implementation and verification of model
  → for prediction of relative ion flux and target erosion

DISCRETE MODEL FOR ENERGETIC ELECTRONS

Trajectories of charged particles without collisions

Lorentz force
acting on particle of charge $q$
from electromagnetic fields $E$ and $B$

$$\mathbf{F} = q\mathbf{E} + q \mathbf{\dot{x}} \times \mathbf{B}$$

+ Newton’s equation of motion
for particle of constant mass $m$

= system of second order ODEs
in terms of components of particle position vector $\mathbf{x}$
to be solved for each particle under consideration

$$\ddot{\mathbf{x}} = \frac{q}{m} (\mathbf{E}(\mathbf{x}) + \mathbf{\dot{x}} \times \mathbf{B}(\mathbf{x}))$$

Assumptions and involved simplifications

- magnetic field induced by current through plasma neglected (Maxwell-Ampere’s law)
  → static magnetic field from permanent magnets computed a priori
- electric field computed a priori from reasonable estimate for number densities (Poisson’s law)
  → allows sequential coupling
  → no self-consistent solution
DISCRETE MODEL FOR ENERGETIC ELECTRONS

Benchmark example - axisymmetric DC magnetron

geometry

results from magnetostatic analysis


$r \approx 19 \text{ mm}; B_z = 0$

from experience known as location of maximum erosion
Benchmark example - axisymmetric DC magnetron
preliminary assessment of trajectories of charged particle species

- electrons released from target
  (secondary electron emission)
- ions created in plasma (ionization)

Electrons confined by magnetic field

$t = 10,000$ ps

$t = 10$ $\mu$s

Ar$^+$ ions not magnetizable due to large gyro-radius
→ falling parallel to electric field lines onto target

- particle trajectories
- unconfined electrons
- magnetic flux density streamlines
Discrete Model for Energetic Electrons

Modeling strategy

Workflow:

- Initialize electron emission flux distribution $j_e(r)$ on target.
- Loop over:
  - Release set of electrons from target based on $j_e(r)$.
  - Integrate electron trajectories.
  - Account for collisions and scattering at random time instants by velocity re-initialization.
  - Project locations of ionization collisions onto target = ion bombardment flux $j_i(r)$.
- Obtain improved electron emission flux distribution $j_e(r) = \gamma j_e(r)$.

Until $j_e(r)$ converged.

electron collision modeling for argon (Ar) as background gas

Collision frequency $\nu$ from total cross section $\sigma$ and scattering angle $\alpha$ from differential cross section $d\sigma/d\Omega$.

![Graph showing electron energy and total cross section](image1)

- 15.8 eV
- 11.6 eV

- $e + Ar \rightarrow e + Ar$ (elastic)
- $e + Ar \rightarrow e + Ar^*$ (excitation)
- $e + Ar \rightarrow 2e + Ar^*$ (ionization)

![Graph showing differential cross section and scattering angle](image2)

- “Fast” electrons: high probability of forward scattering → long lasting confinement.
- “Slow” electrons: isotropic scattering.
Application to benchmark example

electron trajectories in $rz$- and $r\phi$-plane for 3 consecutive runs (after initial 0.1 $\mu$s for 10 electrons)

kink due to collision scattering
Application to benchmark example

integral results after 7 runs over 1.0 µs

normalized ion flux density on target \( j_i(r) \)

Note:
location of maximum ionization flux and target erosion
= location of vanishing normal magnetic field

\[ j_i(r) \approx 19 \text{ mm} \]

estimate for relative target erosion \( \dot{w} \) (normalized by target thickness)

\[ \dot{w} \propto j_i(r) \]
Application to rectangular planar magnetron

estimate of target erosion $w$ (normalized to target thickness of 12 mm) using 5,000 electrons

target utilization: $\sim 18\%$

SUMMARY AND OUTLOOK

Summary

- discrete model for energetic electrons acc. to Sheridan and coworkers
- for prediction of relative Ar+ ion flux and erosion rate
- of planar target in DC sputtering magnetron
- to study design modifications for increased target utilization (ongoing work)
- implemented using COMSOL Multiphysics 4.3a
  - benefit: unified framework, no data exchange
- employed interfaces:
  - B-field:
  - particle trajectories:
  - particle collisions:
  - collision statistics:

Why not DC Discharge (dc)

- computational costs resulting from required spatial and time discretization
- severe anisotropy of mobility/diffusivity tensors
- simple plasma-physics (Ar)

Why not Charged Particle Tracing (cpt)

- collision feature not available in 4.3a (new in 4.3b)
- collision statistics not feasible (even in 4.3b)
- events interface not usable together with particle tracing
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... thanking you for your interest
Application to rectangular planar magnetron

exemplary trajectories of electrons starting at $y = 0$ and $x = 18.5 : 10 : 48.5$ mm over $0.428$ ms (1 rev)