MC-simulation of the metallic flux during magnetron sputtering

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Magnetron sputter deposition simulations

The sputtered particle flux arriving at the substrate:

- Spatial distribution → thickness profile composition
- Energy- and angular distribution → growth mechanism → film properties
  - microstructure
  - crystallographic orientation
  - ...

Knowledge of the arriving flux can be obtained through:

- Measurement (some degree)
- Simulations of the sputter deposition process:
  1) the magnetron discharge
  2) the sputtering from the target
  3) the transport of the sputtered particles through the gas phase
Magnetron sputter deposition simulations

Test particle Monte Carlo (MC)–simulation

Principle :
- The individual trajectories of a large (representative) ensemble of particles are determined.
- A single particle undergoes a sequence of random events (collision), which have a certain probability of occurring.

Advantages :
- accurate: details of the individual collision
- straightforward implementation
- fast

But :
- details about the interaction must be known
- no collective behavior
Simulation overview

Deposition with:

I) Circular planar magnetron

II) Small scale rotating cylindrical magnetron

Required
- for sputtered particles:
  - ejection positions
  - nascent energy and direction
- gas phase transport description
Ejection position: planar target

target erosion $\rightarrow$ a race track

erosion depth proportional to the emission probability at that position

Measure radial erosion profile after experiment
Ejection position: rotatable

Spatial ionization distribution is simulated using a test electron MC-code:

High energy electron trajectories:
- Predefined $\vec{E}, \vec{B}$
  $\Rightarrow$ Lorentz-force
  $$ \frac{d(m\vec{v})}{dt} = q(\vec{E} + \vec{v} \times \vec{B}) $$
- Sputter gas
  $\Rightarrow$ elastic, exciting and ionizing collisions
- Starting positions on target: iteratively
Ejection position: rotatable

Spatial ionization distribution

Projection on target surface, multiply by $I_i = I/(1 + \gamma)$

$I_i$ ion current
$\gamma$ ISEE - coefficient
$I$ total current

Ion current density $j_i$

Introduction
Model
Position
Sputtering
Transport
Metal flux
Spatial
Angular
**Nascent energy and direction**

Sputtering from polycrystalline metal targets by low energy (300-500eV) prolonged bombardment

- Sputter simulation with BCA-package SRIM but: amorphous, flat
  - so: not very realistic

- The nascent angular distribution has a strong influence on the deposition profile. However it is not well known. Solution?
  - decouple nascent energy and direction
  - nascent energy distribution: Thompson

\[
\frac{dY}{dE_1} \propto \frac{E_1}{(E_1 + U_S)^3}
\]

- \(U_S\): surface binding energy

- assume nascent angular distribution to be a fitting function

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**Understanding the Deposition Profile**

The nascent energy and direction of sputtered particles play a crucial role in determining the deposition profile during sputtering processes. Low energy bombardment, typically in the range of 300-500 eV, can affect the angular distribution and energy of the sputtered particles, which in turn influences the deposition characteristics on the target or substrate.

Sputter simulations, such as those performed with the SRIM software package, are commonly used to model these processes. However, the assumption of an amorphous, flat deposition profile made by SRIM may not always be realistic, especially in cases where the material properties or the bombarding conditions require a more sophisticated approach.

The nascent angular distribution, which refers to the direction of the sputtered particles as they leave the target, has a significant impact on the deposition profile. The manner in which these particles are directed can lead to variations in the thickness and composition of the deposited layer. Understanding and controlling this distribution is therefore key to optimizing the sputtering process and achieving desired outcomes.
Gas phase transport

Assumptions:

- sputtered particles are neutral atoms
- only elastic collisions with neutral gas atoms
  - ionization degree \( \ll 1 \)
  - density of sputtered particles \( \ll \) density of gas atoms
- background gas: homogeneous and in thermal equilibrium
  \( \rightarrow \) gas rarefaction is not taken into account.

\( \Rightarrow \) sputtered particles follow a sequence of straight trajectories, each ended by a binary and elastic collision.
Gas phase transport

Individual collision:

Centre of mass description

Polar angle $\theta_{\text{com}}$

- classical scattering theory $\theta_{\text{com}} (E_{\text{com}}, p)$
- $p \rightarrow$ random

Azimuthal angle $\phi_{\text{com}} \rightarrow$ random

Interaction potential $V(r)$

1) screened Coulomb potentials
2) quantum chemical potential for Cu-Ar and Al-Ar

Advantage: model low energy attractive interaction

+ gas motion $\rightarrow$ better description of (near) thermal flux

Gas phase transport

Required:

1. free path \( \lambda = -\lambda_m \ln(RN) \)
2. post collision velocity

Gas atoms:
Maxwellian velocity distribution
\( 3/2k_B T \approx 0.04 \text{eV}, \) most probable speed \( v_p \)

Sputtered atoms: 100 - 0.04 eV, speed \( v_s \)

Accuracy and computational speed

I) \( v_s > 5 v_p \) stationary gas atoms

II) \( v_s < 5 v_p \) with gas motion
optional

III) \( 1/2 m_s v_s^2 < 3/2k_B T \) thermalized
Deposition rate distribution rotatable magnetron

Measure deposition rate with a quartz crystal microbalance for:
- Cu, Ti, Al target
- Ar pressure: 0.3, 0.6 and 1 Pa

as function of $\theta$ at:
- 3 radial distances: $r_1, r_2, r_3$
- 3 z-positions: $z_1, z_2, z_3$

$\Rightarrow$ Outward radial metal flux $(r, \theta, z)$

Compare to simulation

Example:

Al, 0.3Pa Ar
$r = r_2$, $\theta = -30^\circ$, $z = z_2$
$V_d = 357$ V, $I = 0.45$ A
Deposition rate distribution rotatable magnetron

\[ \frac{d^2 Y}{d^2 \Omega} (\theta) = \sum_{i=1}^{5} c_i \cos^i \theta \]

Fit coefficients \( c_i \) from the simulated deposition profiles of an angular base set.

- Lowest pressure, shortest distance
- Minimal scattering
- SRIM: almost cosine so Cu < Ti < Al

P = 0.3 Pa

\( r = r_1 \)
Deposition rate distribution rotatable magnetron

Heart-like emission
Deviation from cosine Cu->Al->Ti

SRIM: amorphous, flat
non-cosine emission due to:
- target crystallinity
- surface roughness
Deposition rate distribution rotatable magnetron

Pressure dependence:

\[ r = r_1 \]
\[ Z = Z_2 \]

Radial dependence:

\[ P = 0.6 \text{ Pa} \]
\[ Z = Z_1 \]
Angular distribution arriving metal flux

Measurement with a metal flux monitor\(^1\)

Working principle: pinhole camera

Compare the deposition profile in the monitor to simulations

Example:

\text{Cu – Ar}

\text{Planar target}

\text{Monitor}

central above distance: 9.5 cm

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Thanks for the attention

SIMTRA - Simulation of Metal Transport

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Version 2008 (1)
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Simulation code:
www.draft.ugent.be

Group picture

Not a zoo you say?