Highlights in modeling the reactive magnetron sputtering process with RSD2013

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RSD2015
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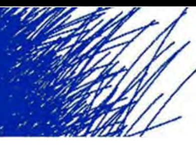
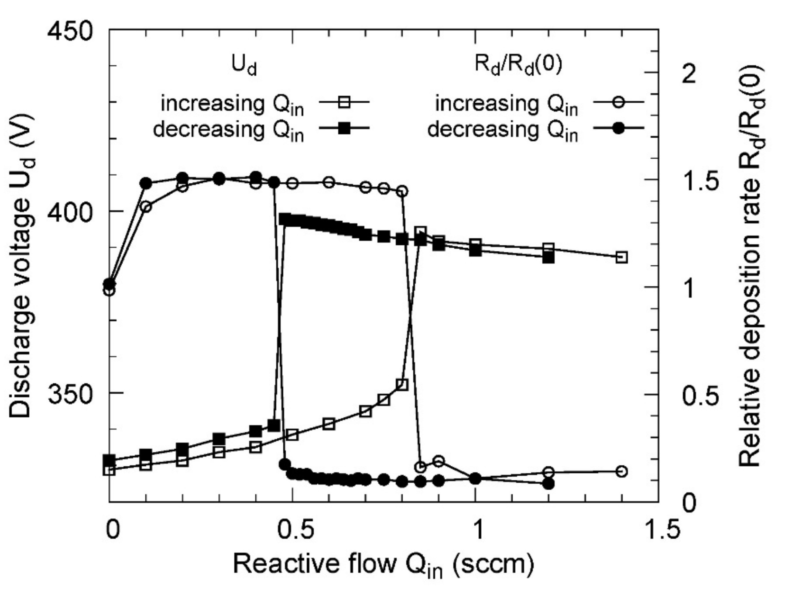
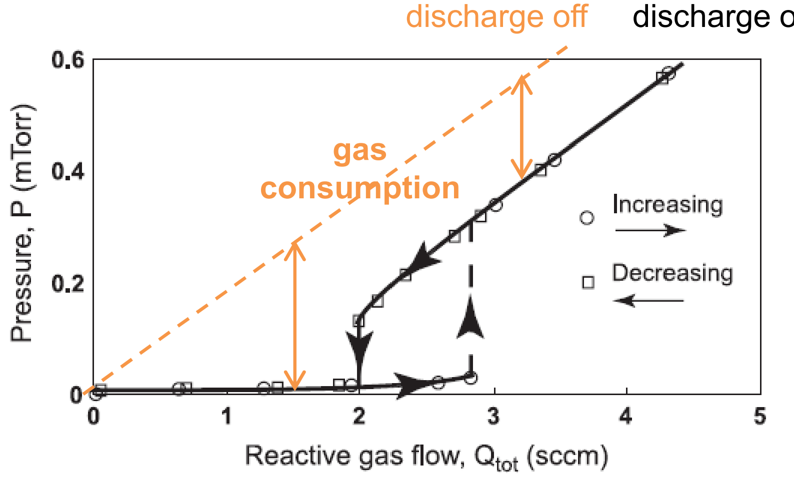
Outline

1. Introduction
2. RSD2013 model
3. Finding parameters
4. Case studies
   a) Redeposition
   b) Dual target
   c) Substrate rotation
5. Conclusion



Hysteresis phenomena





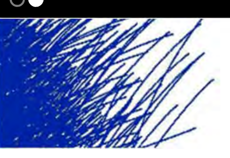
Direct controlled hysteresis experiment = stepwise in/decrease of single **operation parameter** (e.g. reactive flow Q_{in})

Hysteresis in

a) reactive gas pressure
b) discharge voltage
c) deposition rate

by **poisoning** (=compound formation target)

a) vanishing getter pump
b) changing Y_{SEE}
c) decreasing sputter yield ($Y_c << Y_m$)

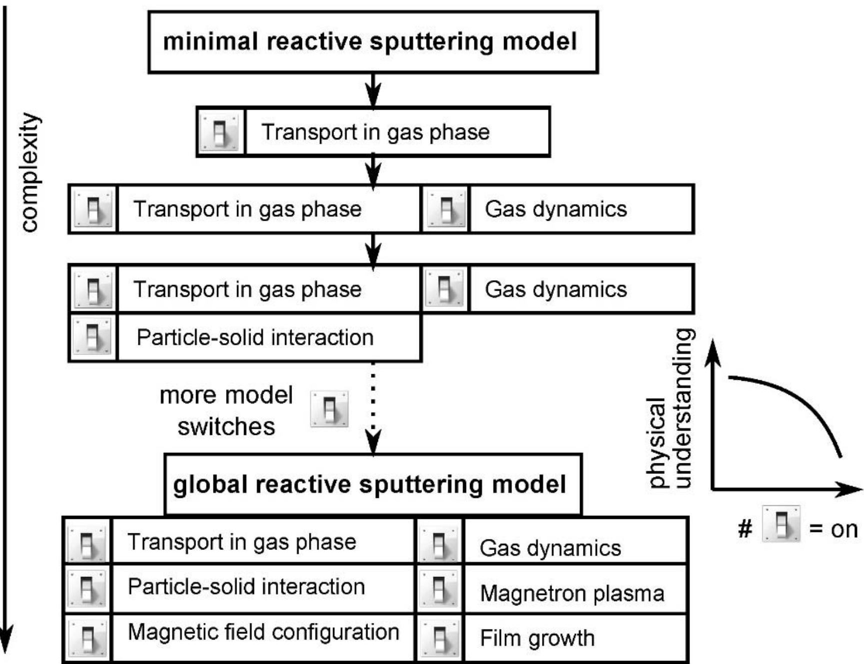


Two modeling approaches

Atomistic approach =
combine complex but detailed models of the subprocesses into a even more complex global model

Holistic approach =
start from a minimal but global model that is gradually expanded with the ability of modularity to a complex global model

complexity
global reactive sputtering model
Particle-solid interaction
Film growth
Magnetic field configuration
Magnetron plasma
Gas dynamics
Transport in gas phase
physical understanding



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Variables in RSD model

System part	Resolved variable		Model approach
Chamber	P Q_p	reactive partial pressure gas flow to pump	one-cell
Target •Surface • Subsurface	Q_t θ_m θ_c θ_r $n_m(x)$ $n_r(x)$	gas flow consumption metallic fraction chemisorbed fraction reacted fraction metal concentration reactive gas concentration	one-cell uniform current multi-cell non-uniform current depth profile SRIM implantation
Substrate	θ_s Q_s	chemisorbed fraction gas flow consumption	one-cell multi-cell SIMTRA profile

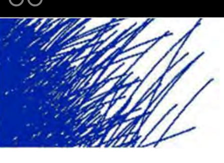
5 BALANCE equations ⬄ 5 ODE's

$$0 = f(y) \leftrightarrow \frac{dy}{dt} = f(y)$$

Steady state ⬄ Time

2 ODE's ⬄ 2 PDE's

$$0 = f\left(y, \frac{\partial y}{\partial x}\right) \leftrightarrow \frac{\partial y}{\partial t} = f\left(y, \frac{\partial y}{\partial x}\right)$$



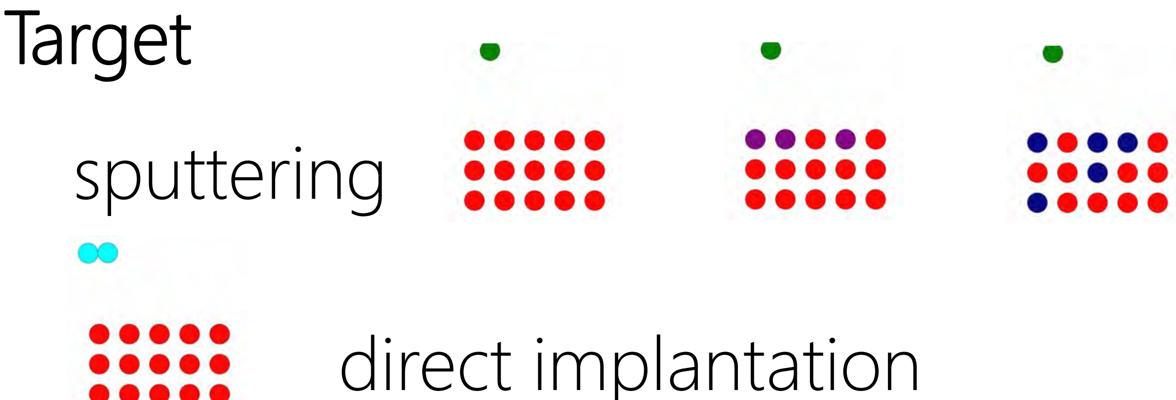
Processes in RSD2013

Target

sputtering

metal M
chemisorbed MR_z
reacted MR_z
reactive molecule R_2
inert gas Ar
reactive implanted atom R

Processes in RSD2013



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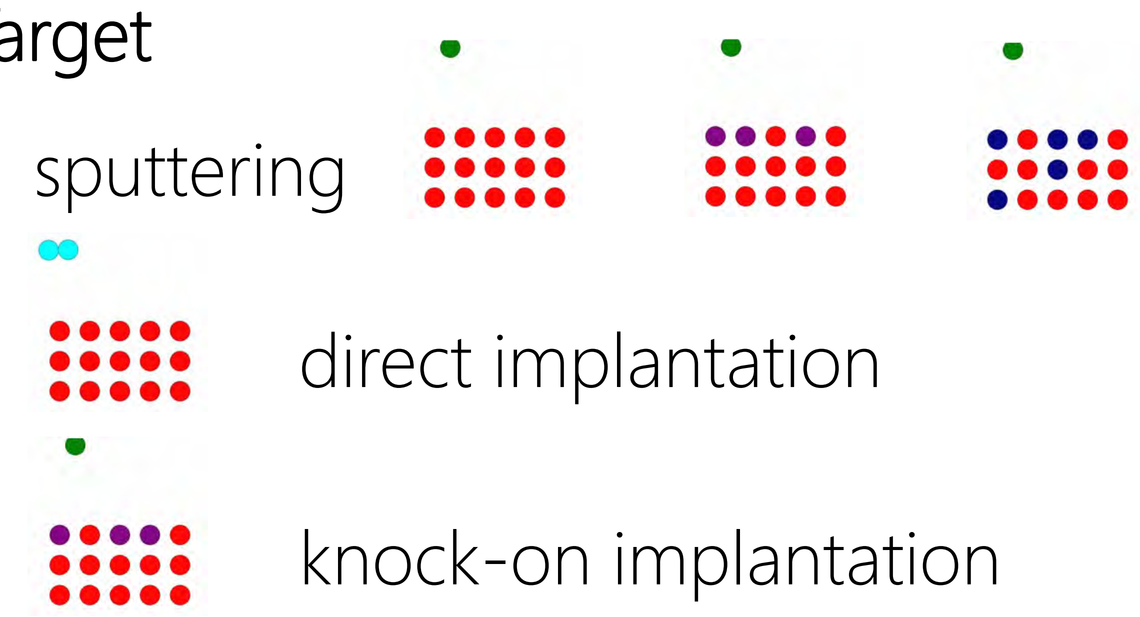
Processes in RSD2013



- metal M
- chemisorbed MR_z
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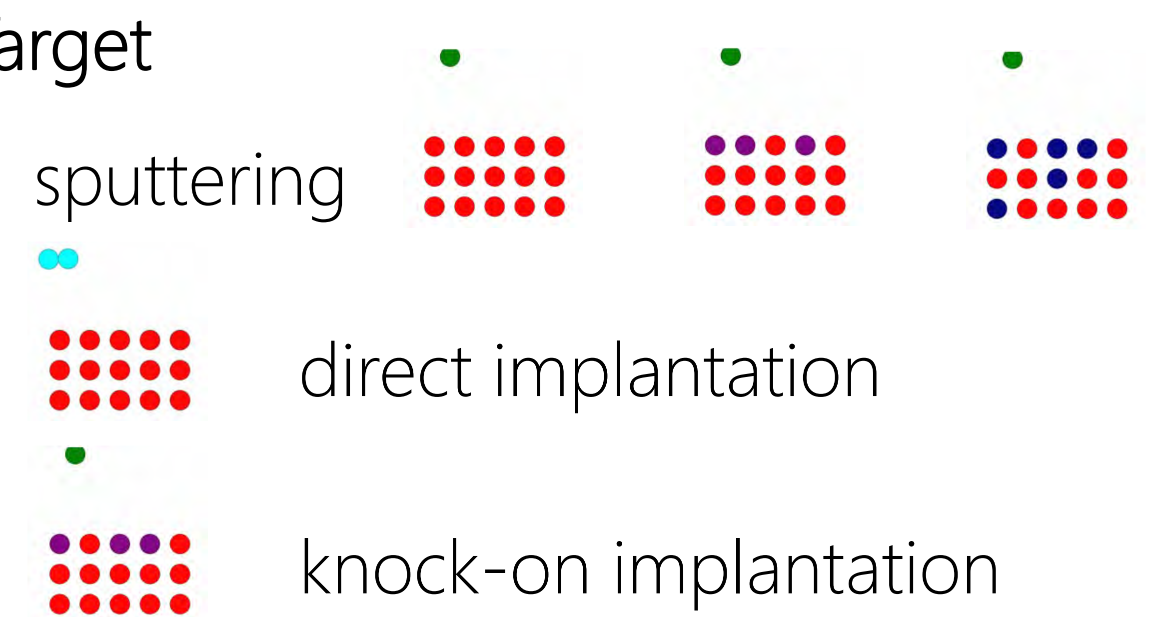
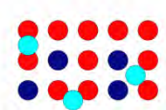
Processes in RSD2013



reaction



- metal M
- chemisorbed MR_z
- reacted MR_z
- reactive molecule R_2
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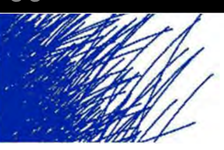
- reactive implanted atom R



Processes in RSD2013

Target

sputtering

direct implantation

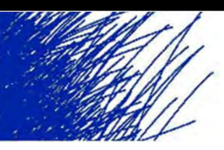
knock-on implantation

reaction

Target & substrate

deposition

- metal M
- chemisorbed MR_z
- reacted MR_z
- reactive molecule R_2
- inert gas Ar
- reactive implanted atom R



Processes in RSD2013

Target

sputtering

direct implantation

knock-on implantation

reaction

Target & substrate

deposition

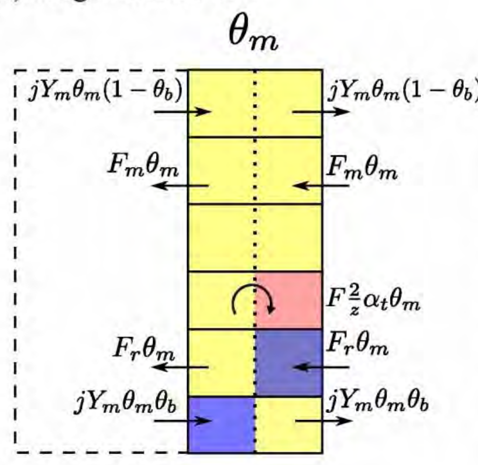
chemisorption

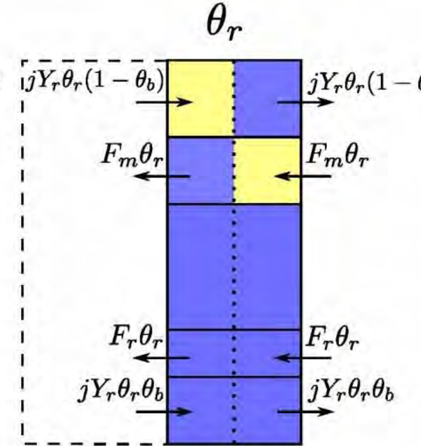
- metal M
- chemisorbed MR_z
- reacted MR_z
- reactive molecule R_2
- inert gas Ar
- reactive implanted atom R

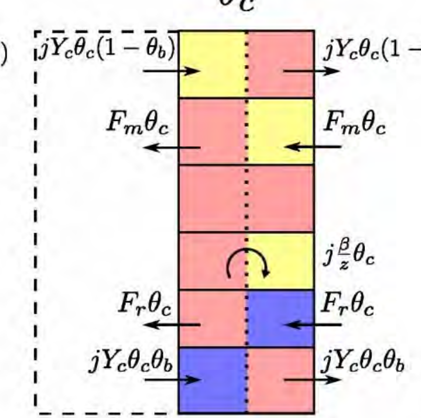
From RSD2009 to RSD2013

(a) Target surface cell

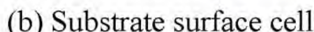
Derivation based on conservation of particles M and MR_z

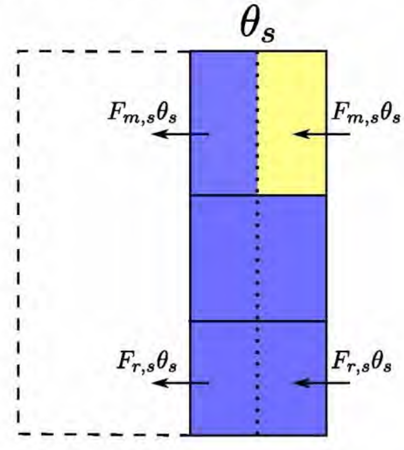


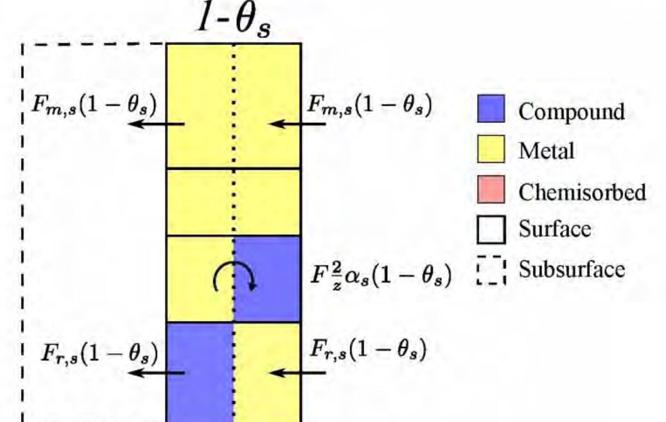




multi-cell target with deposition = **redeposition**



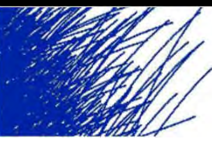




RSD2013 = critical revision of RSD2009

- two discrete layer + subsurface
- saturation limit
- redefining surface equations

K. Strijckmans et al., *J. Phys. D: Appl. Phys.* 47 (2014) 235302



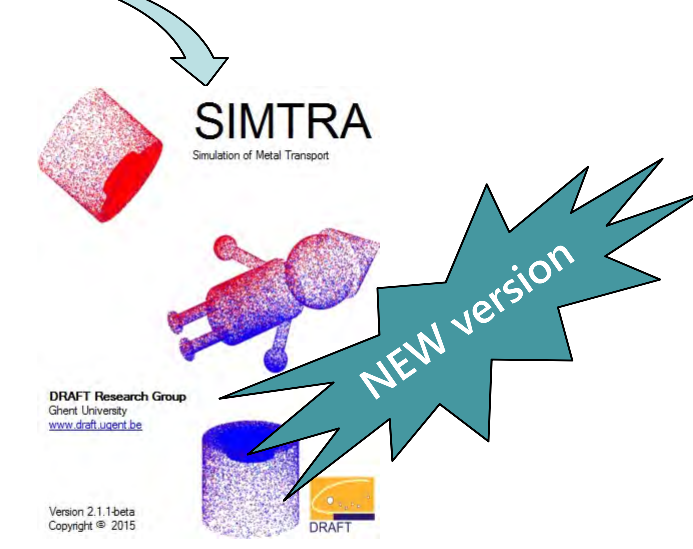
Connected with other software

OR

SDTrimSP

TriDyn

nascent distribution



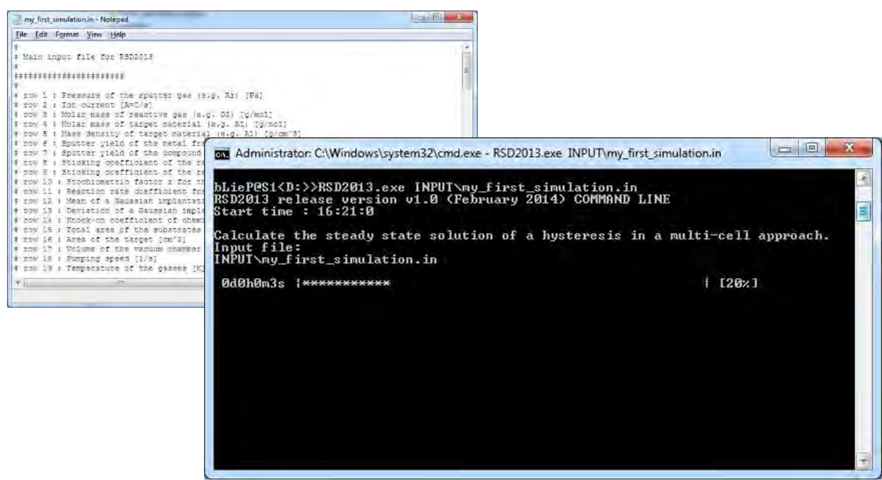
reactive implantation profile
knock-on yield
(sputter yields ?!)

(re)deposition profile
redeposition fraction

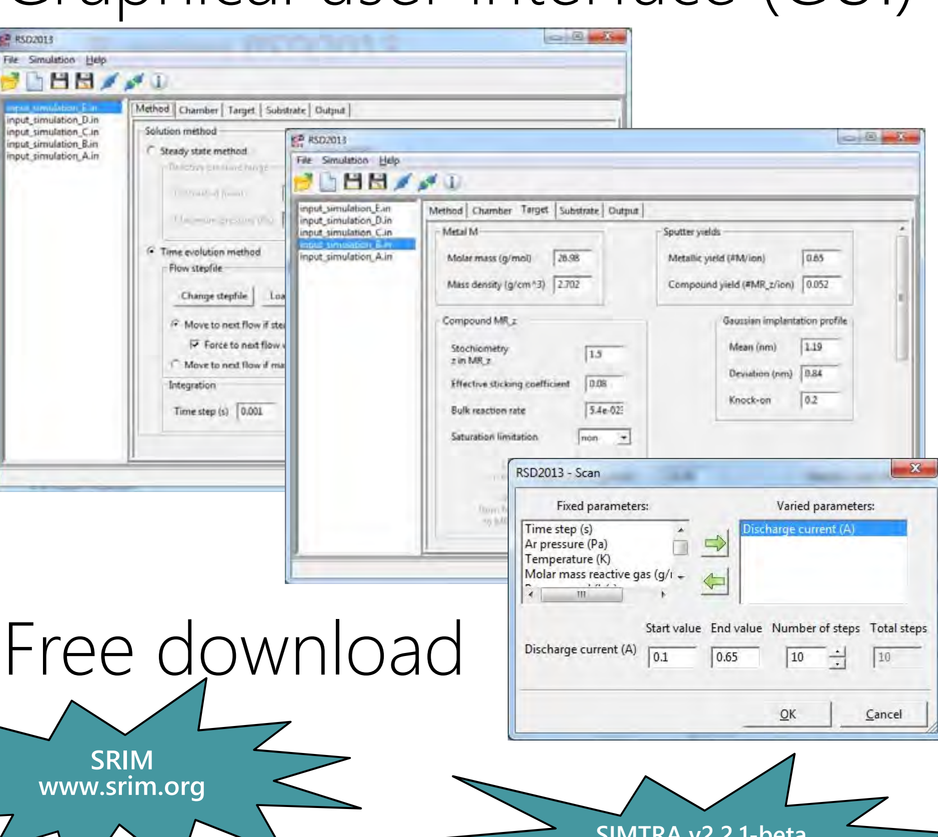
D. Depla, et al.,
Thin Solid Films 520(20), 6337 (2012)

Running RSD2013 software

Command line



Graphical user interface (GUI)



Manual

Installation

The RSD2013 software is compiled to run on a Windows platform. It mainly consist out of two executables: RSD2013_GUI.exe and RSD2013.exe. The first executable is the graphical user interface (GUI) which creates the input files and can start up the RSD2013 simulations. The second executable is the effective simulation program. After generating an input file with the GUI or manually, you can run RSD2013_GUI.exe on the command line to perform the simulation.

Installation of the RSD2013 software is easy. Simply unpack the compressed zip file to a location of your choose and you are ready to use the software. The directories icons and templates should be left intact. Renaming the RSD2013.exe executable will make running simulations through the GUI impossible.

Overview

The RSD2013 software is developed to simulate the reactive sputter process of a DC magnetron. It's focus is on the possible hysteresis curve of this process. To this end, it solves the equations of the RSD2013 model, as can be found in following reference. The nomenclature of the variables used here corresponds with the one of this reference.

The RSD model calculates following variables:

- the pressure P_r of the reactive gas in the system
- the compound θ_r, chemisorbed θ_c and metal θ_m fractions of the target surface
- the compound θ_s and metal fractions of the substrate surfaces
- the metal concentration n_M in the target subsurface region
- the compound concentration in the target subsurface region which is directly derived from n_M
- the non-reacted implanted reactive gas concentration n_R in the target subsurface region
- the consumptions Q_t of reactive gas by the target
- the consumptions Q_s of reactive gas by the substrate
- the amount of reactive gas Q_p pumped away by the vacuum pump
- the amount of reactive gas Q_{in} introduced into the vacuum chamber

To this end the RSD model needs several input variables. These input variables are clarified throughout the following sections.

Quick start

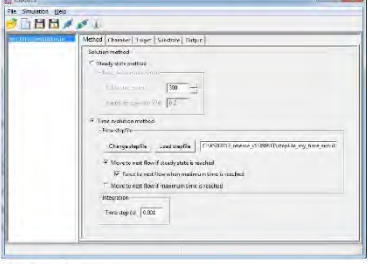
To run a first RSD simulation, you just double click the GUI executable RSD2013_GUI.exe. By default a complete input is specified in the window tabs Method, Chamber, Target, Substrate and Output.

All simulation options are visual within the window tabs. None used or relevant options or fields are grayed out and unaccessible. They become (un)accessible depending on which simulation choices you make. For example, when choosing the Steady state method in the window tab Method as solution method, then the fields connected to the Time evolution method are irrelevant and as such grayed out.

Most fields have a restricted range of values that can set. This restriction only applies to the GUI and can be easily overruled by manually editing the input files.

Method

The window tab Method basically specifies how the RSD2013 model should be solved. As solution method, two option are available the Steady state method and Time evolution method. Evidently is the choice between the two methods exclusive.



Method window tab.

Steady state method

To solve the RSD2013 model in its steady state description. The reactive pressure P_r is stepwise increased up to the Maximum pressure and subsequently decreased. The total number of reactive pressure P_r values that are calculated are given by the field Calculated points.

Calculated points

To define the total number N of reactive pressure P_r values that are calculated in the Steady state method. So the $N/2$ reactive pressure P_r values are each calculated twice. The first time for an increasing reactive flow Q_{in} and the second time for a decreasing reactive flow Q .

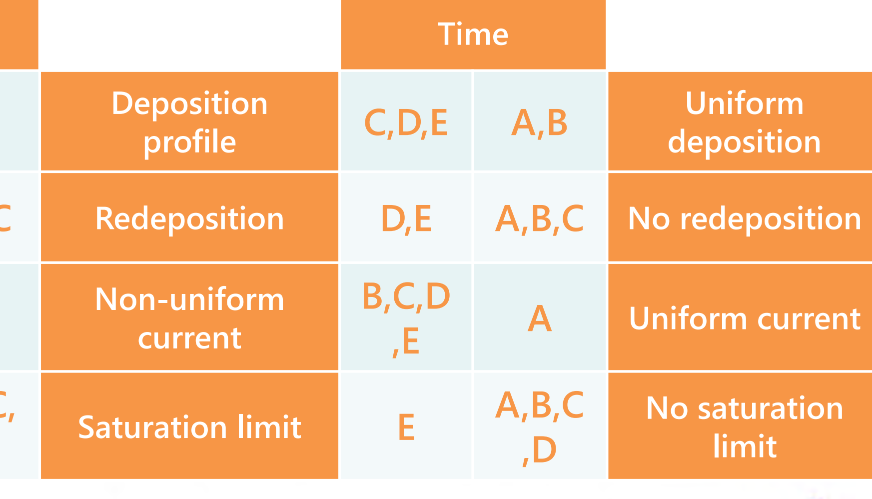
Free download

SRIM
www.srim.org

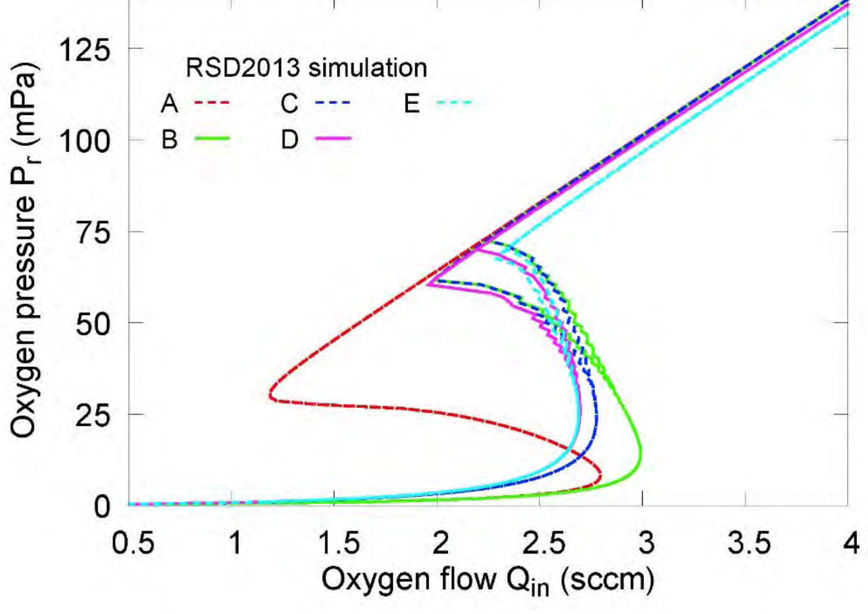
RSD2013 v1
www.DRAFT.ugent.be

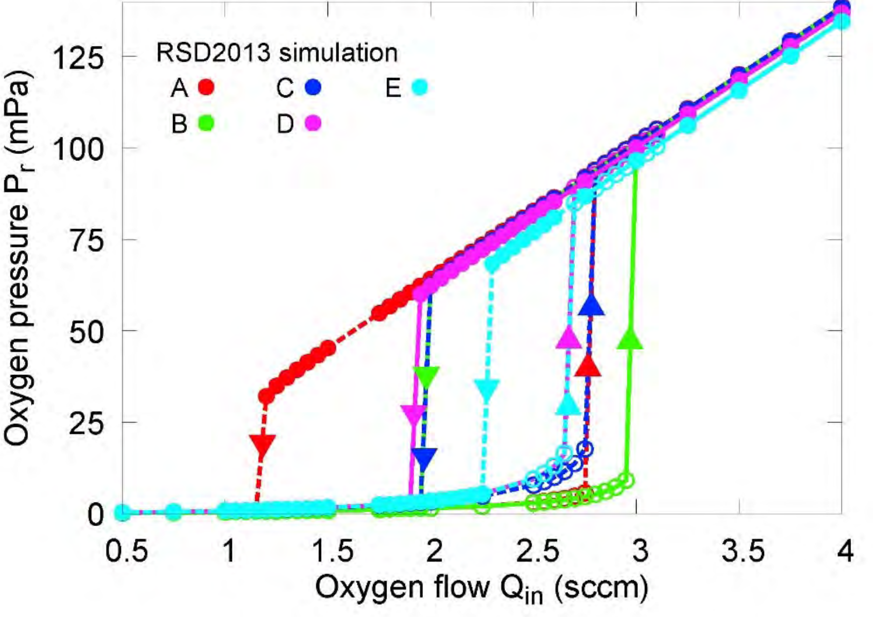
SIMTRA v2.2.1-beta
www.DRAFT.ugent.be

The “Chinese menu card” of RSD2013



Solution:	Steady			Time		
Uniform deposition	C,D,E	A,B	Deposition profile	C,D,E	A,B	Uniform deposition
No redeposition	D,E	A,B,C	Redeposition	D,E	A,B,C	No redeposition
Uniform current	B,C,D,E	A	Non-uniform current	B,C,D,E	A	Uniform current
No saturation limit	E	A,B,C,D	Saturation limit	E	A,B,C,D	No saturation limit





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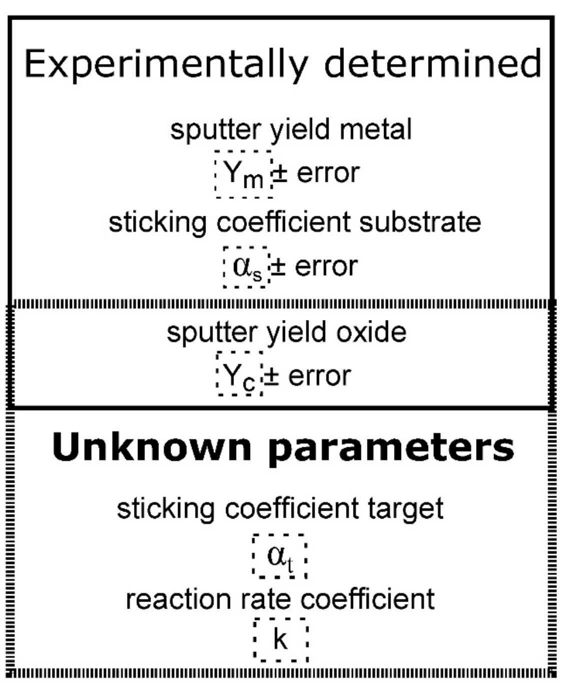
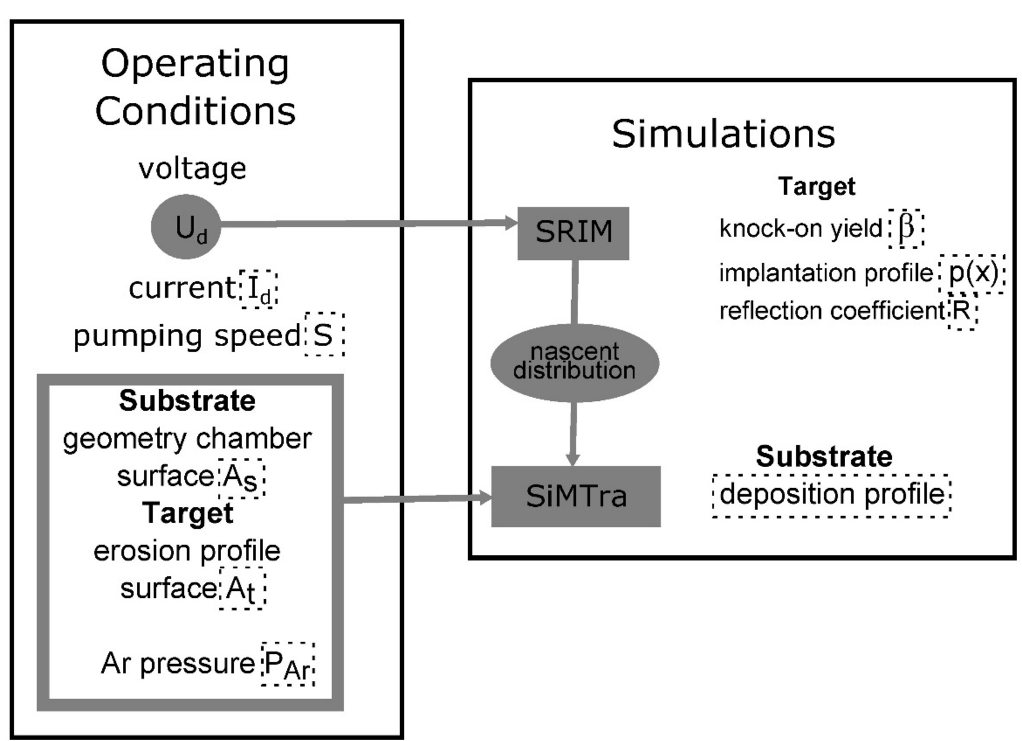
Input parameters : the quest



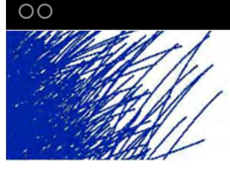


Problem: 2 unknown parameters (α_t, k)

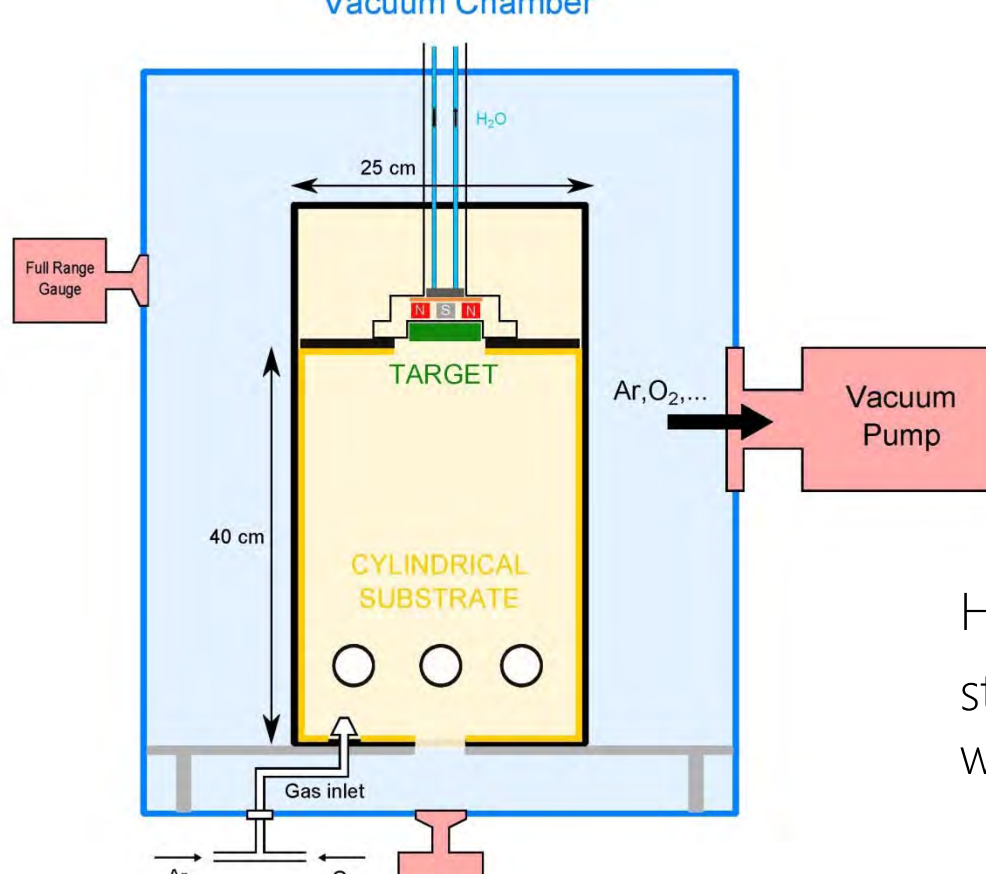
Reason: experimentally or by simulation hard to retrieve (even for Y_c)

Goal: fit freedom and material dependency

Solution: fitting RSD model to experiments



Experimental setup



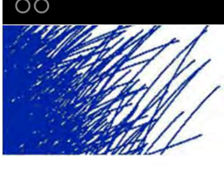
Sputter conditions:

- Target Al or Y (D = 2")
- Process gas Ar
- Reactive gas O_2
- S = 55 L/s or 112 L/s
- P_{base} = ~10^{-4} Pa
- P_{Ar} = 0.45 Pa or 0.37 Pa
- I = 0.4 A, 0.5 A or 0.6 A

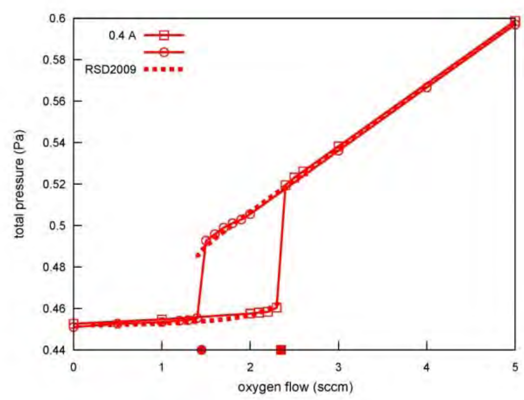
Hysteresis experiment =

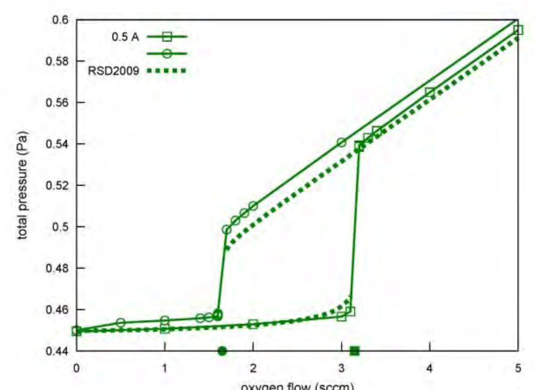
stepwise in/decreasing the O_2 flow while collecting

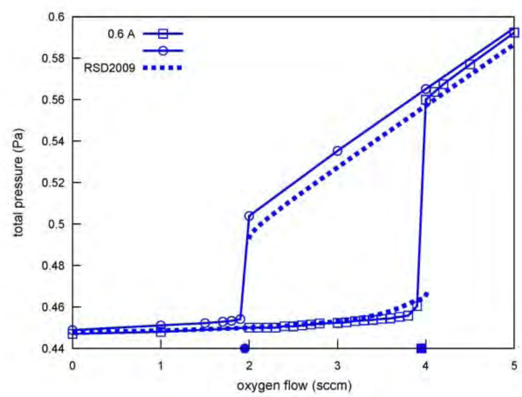
👌 steady state values 👌
V, I and P_{tot}



Fitting procedure





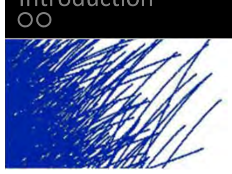


Fit criteria = 6 critical O_2 flow values

- goodness of the fit = worst match out of 6
- fits are 'good' if critical points fall within **acceptance tolerance f_a** (=experimental resolution)

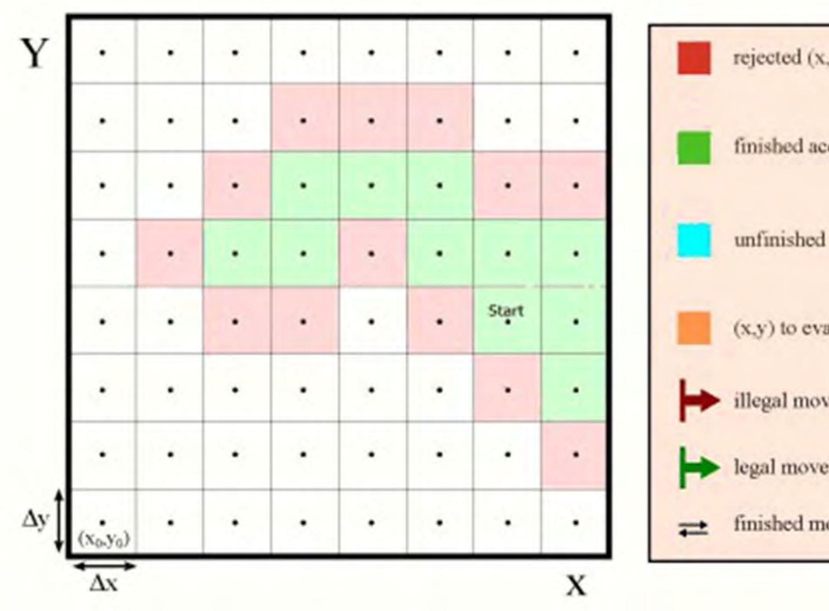
Simulation includes

✓ measured V and I variation	Y_m and I_{ion}
✓ changing target oxidation	oxygen implantation profile
	I_{ion} (by Y_{SEE})



Scan algorithm

Serial implementation illustrated for a 2-D parameter space (X,Y)



Goal finding all (x_i,y_i) combinations that pass the fit criteria

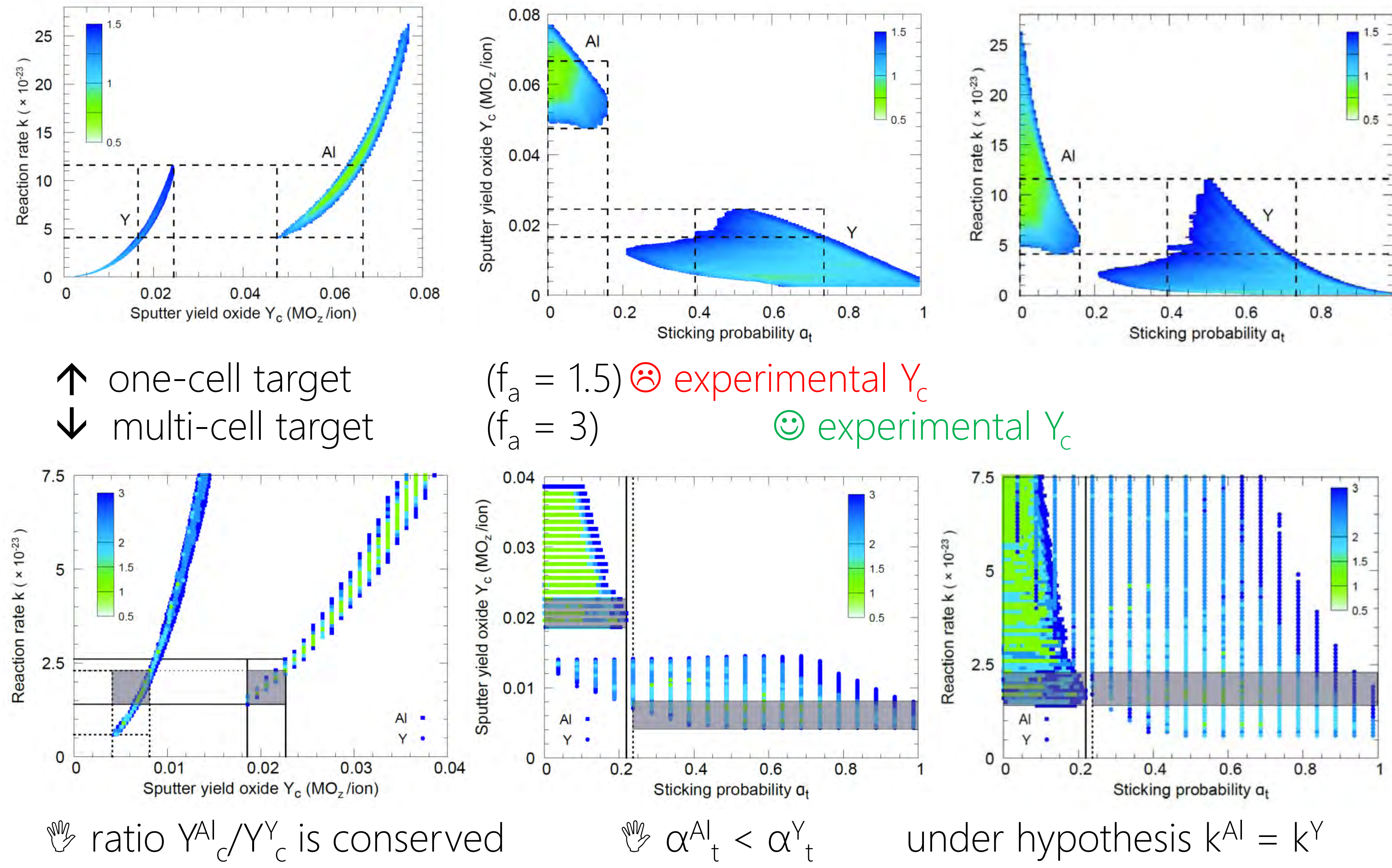
Ingredients

- starting point (**Start**) ➔ found by (slightly) modified version
- step size (**Δx**, **Δy**)
- parameter boundaries
- fit procedure + acceptance tolerance f_a (>1)
- three lists: rejected, accepted and unfinished

Limitation only for a connected region

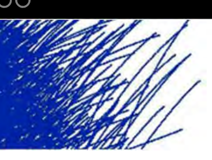
K. Strijckmans, et al., *Surf. Coat. Technol.* 206 (2012) 3666

Fitting results : correlations

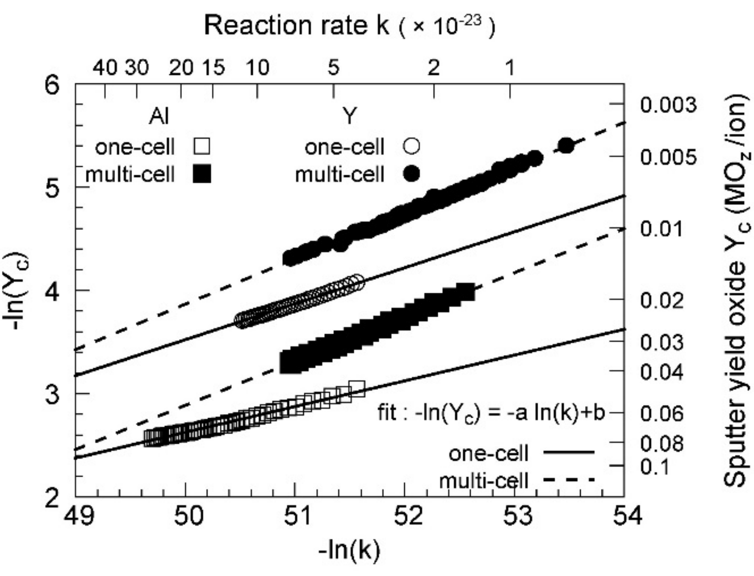


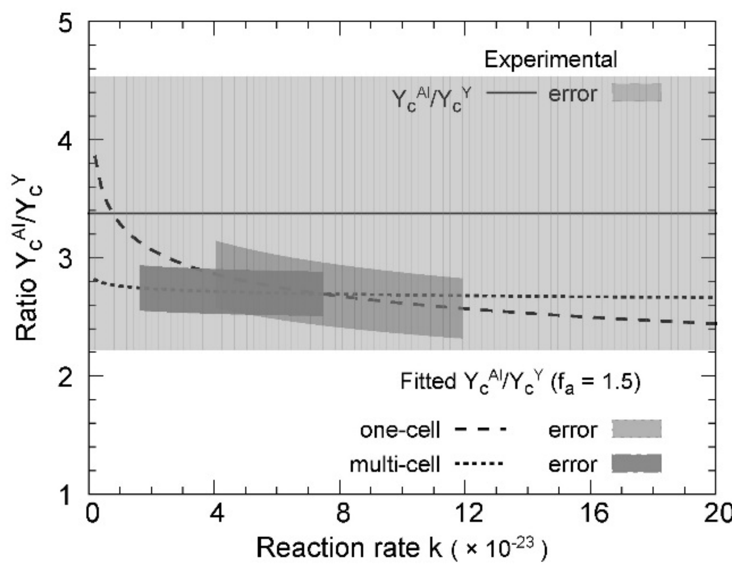
ratio Y^{Al}_c/Y^{Y}_c is conserved

$\alpha^{Al}_t < \alpha^{Y}_t$ under hypothesis $k^{Al} = k^{Y}$



Fitting results : analysis



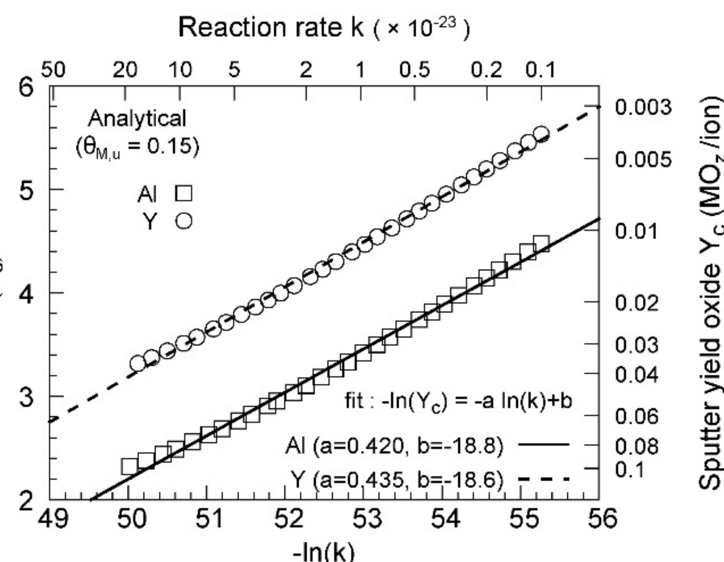


Reaction coefficient k and sputter yield oxide Y_c highly correlated

➔ Power law $Y_c = b' k^a$

✍ ratio Y^{Al}_c/Y^{Y}_c and correlation independent of

- reaction coefficient k
- one-cell or multi-cell target
- implantation profile



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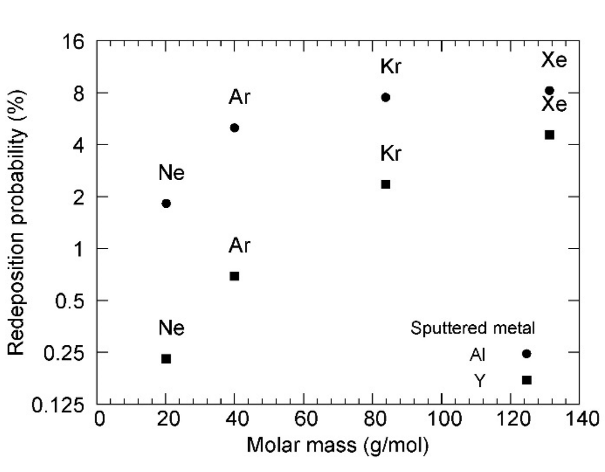
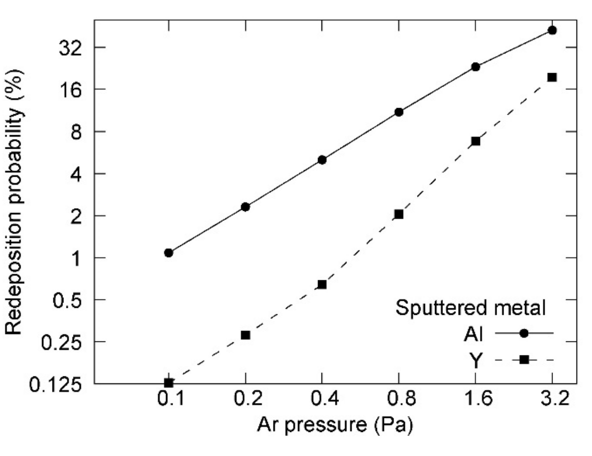
Case study : redeposition

Redeposition influenced by

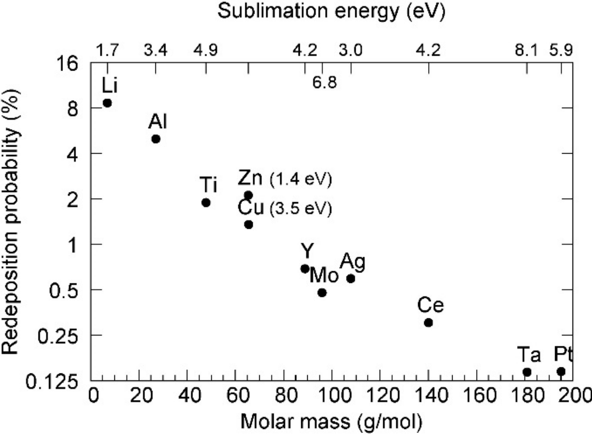
1) sputter gas

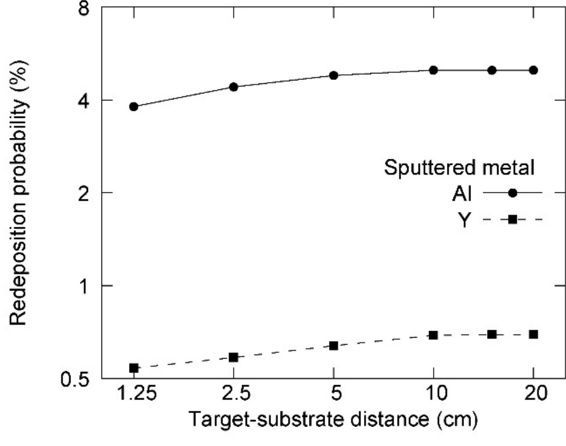


2) gas pressure



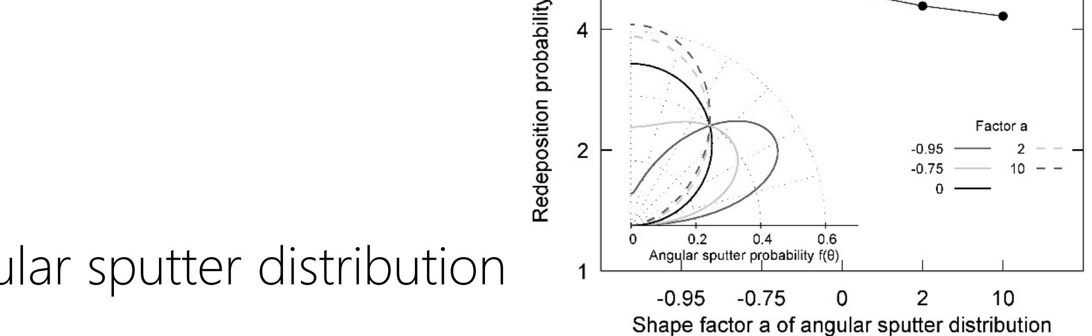
3) sputtered element



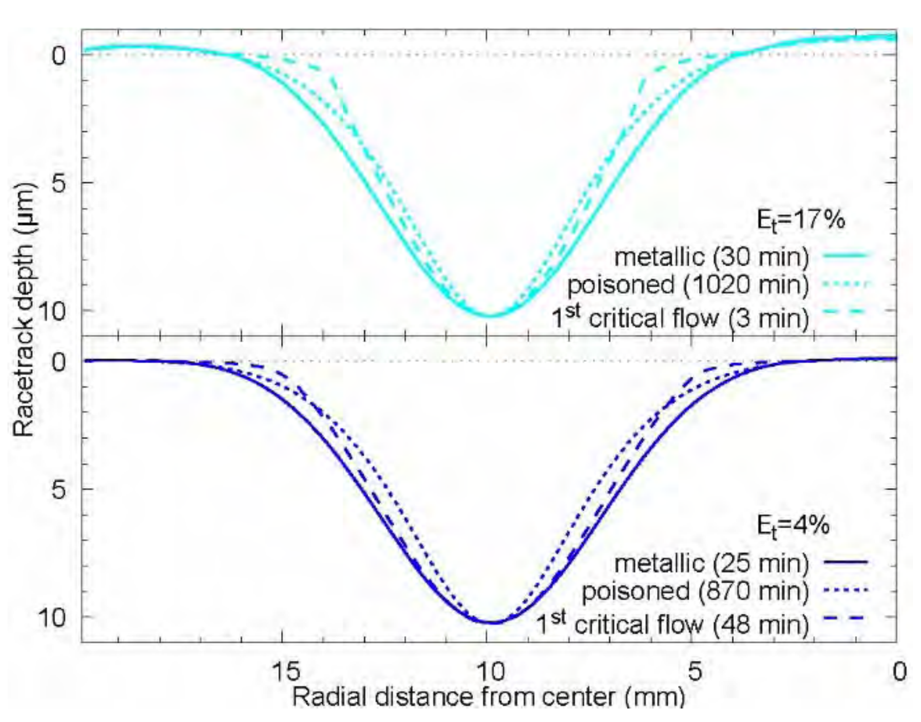


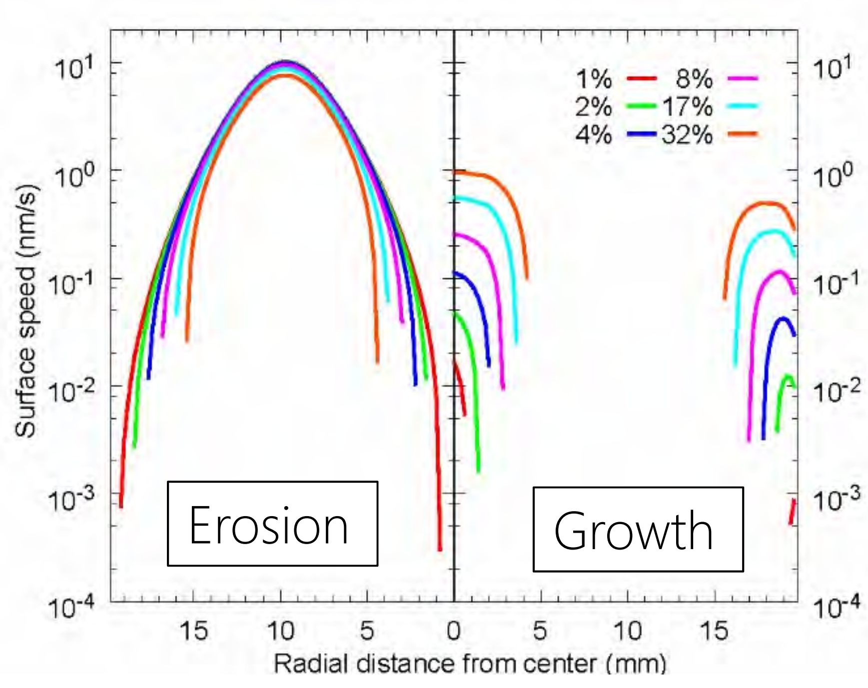
4) target-substrate distance

5) angular sputter distribution



Redeposition: Effect on racetrack profile





Shape of racetrack depends

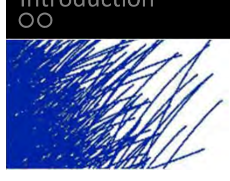
- redeposition fraction
- operation point

Increasing redeposition fraction decrease zone of effective erosion.

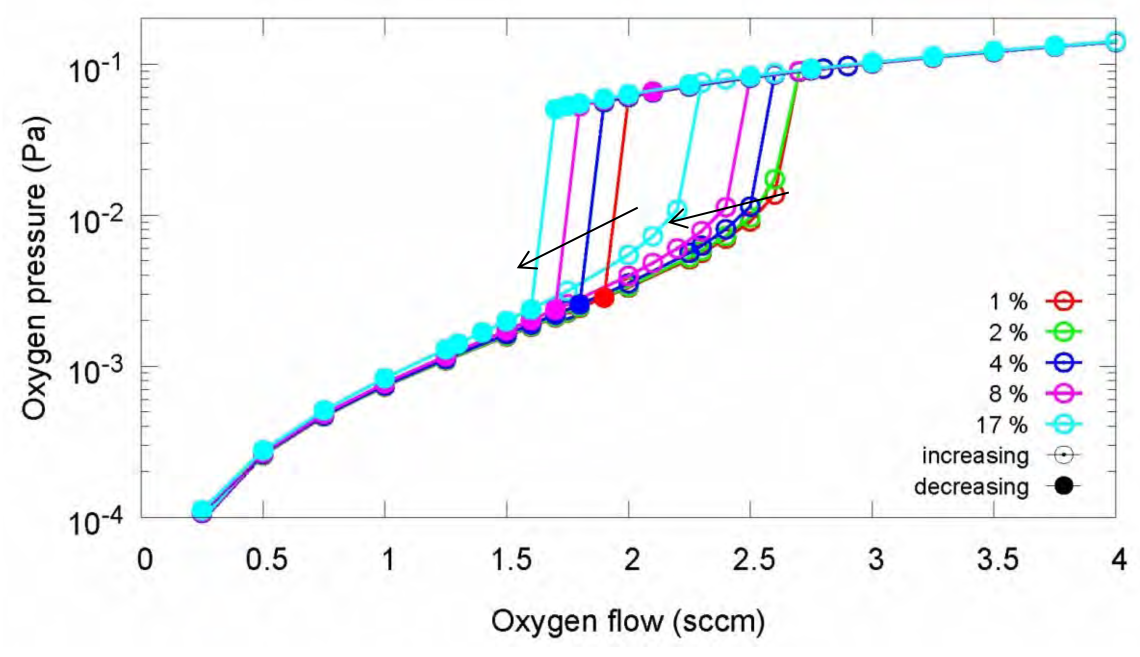
Surface speed v_s measure for racetrack depth

$$D = v_s \, \Delta t$$

K. Strijckmans, et al., *Appl. Surf. Sci.* 331, 185 (2015)



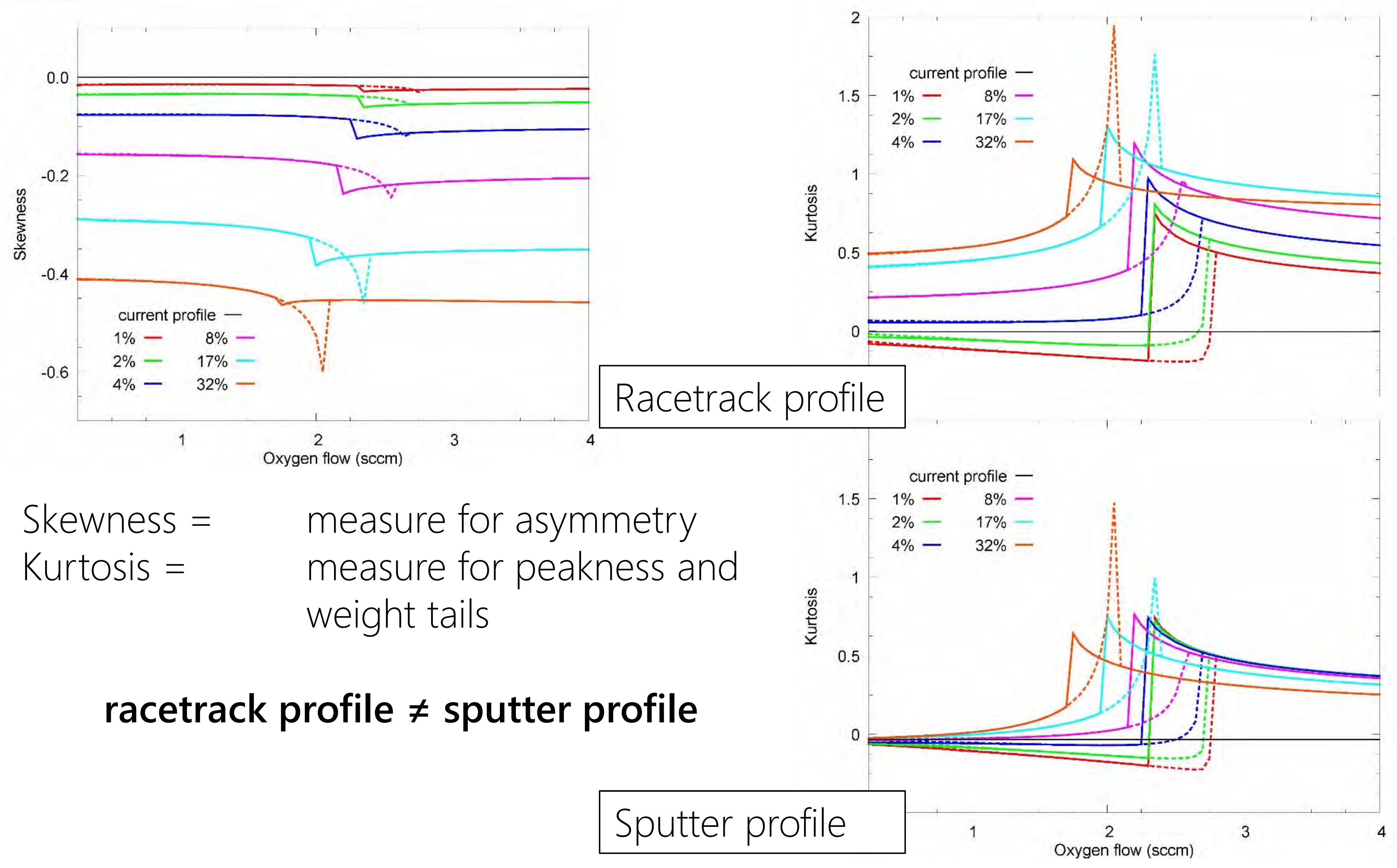
Redeposition: Effect on critical points



Shifting of both critical points to lower oxygen flows.

- 1st critical point:
  the redeposition acts as a sink for sputtered metal
  it reduces the metal flux towards substrate, which more easily gets oxidized
- 2nd critical point:
  the redeposition slows down the erosion which give more time for reaction

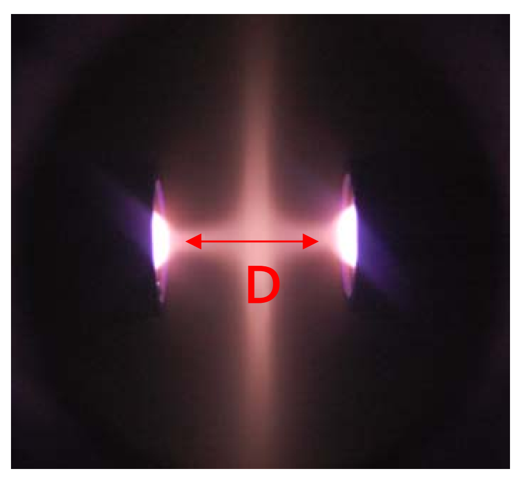
Redeposition : Shape modifications



Outline

1. Introduction
2. RSD2013 model
3. Finding parameters
4. Case studies
   a) Redeposition
   b) Dual target
   c) Substrate rotation
5. Conclusion

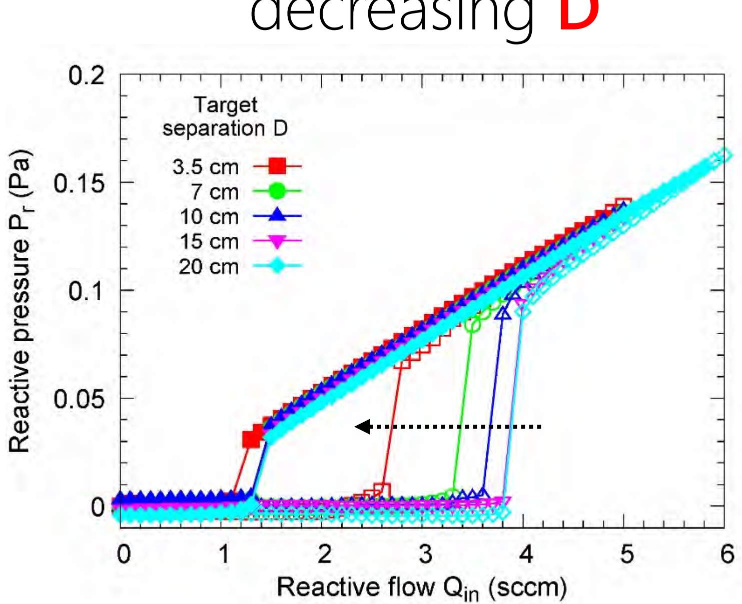
Dual target : hysteresis experiment



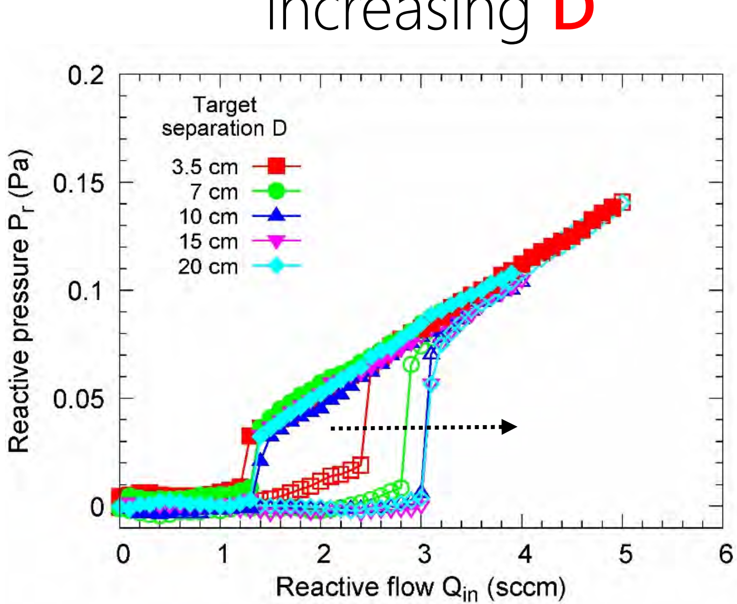
Conditions:

- cuboid chamber (50 x 50 x 50 cm)
- two facing 2″ circular Al targets
- gasses Ar (0.4 Pa) / O_2
- target separation **D** 3.5 to 20 cm
- pumping 55 Ls^{-1}
- discharge current 0.3 A

decreasing **D**

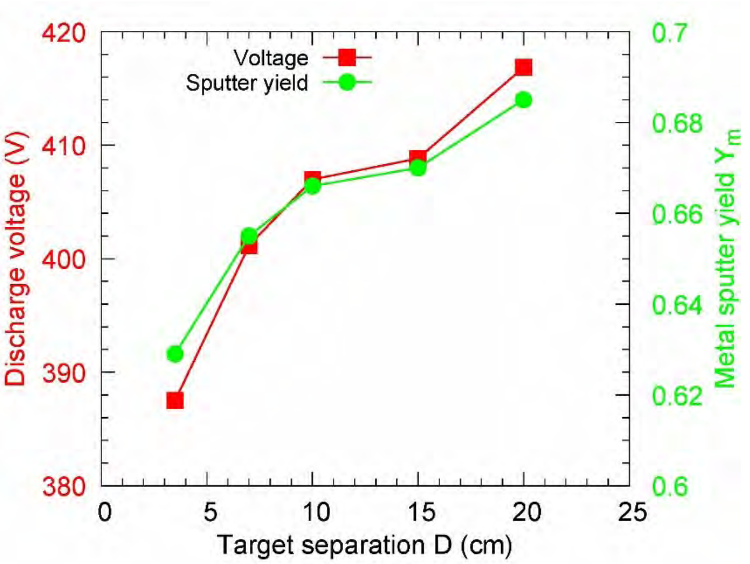


increasing **D**



Dual target : target erosion

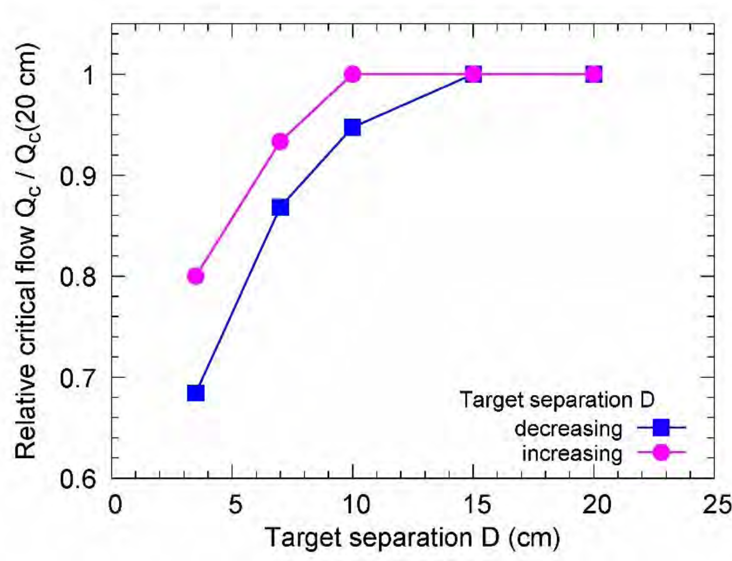
decreasing **D**



target erosion amplifies
shift 1st critical point

target thickness ↘
magnetic field ↗
voltage ↘
sputter yield ↘

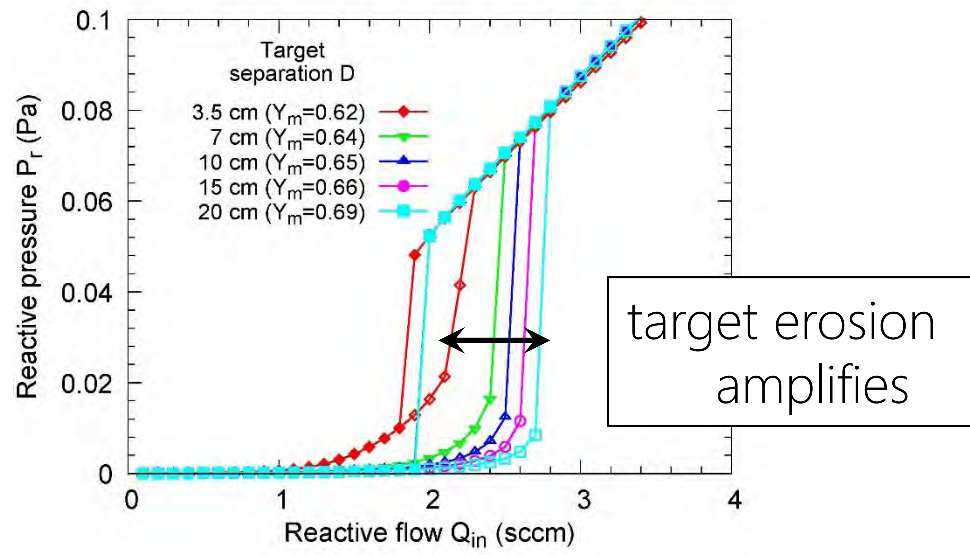
in/decreasing **D**



decreasing **D** ➢ erosion amplifies
increasing **D** ➢ erosion relaxes

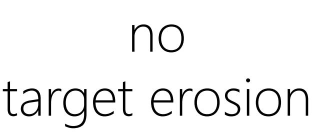
1st critical point shifts ↘

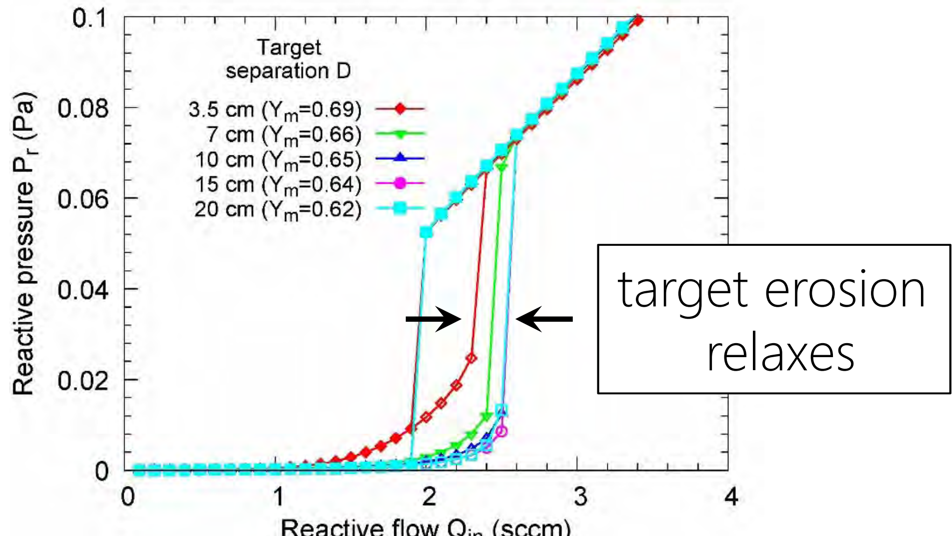
Dual target : RSD simulation

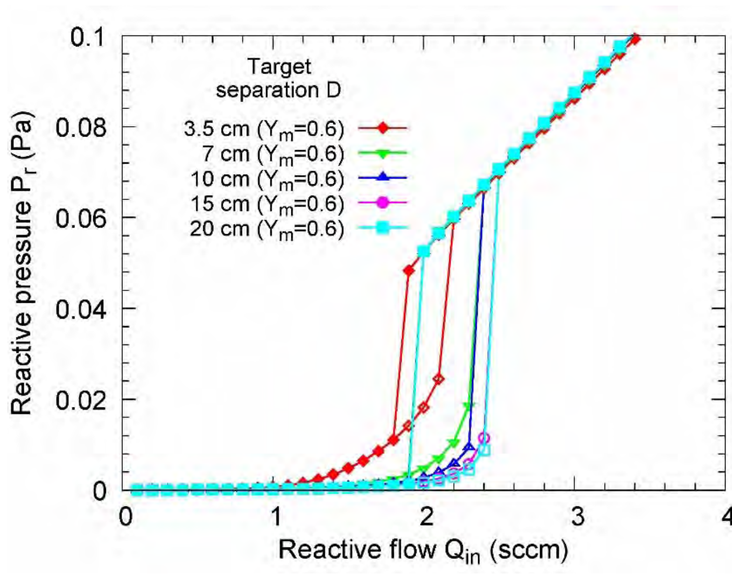


Conditions:

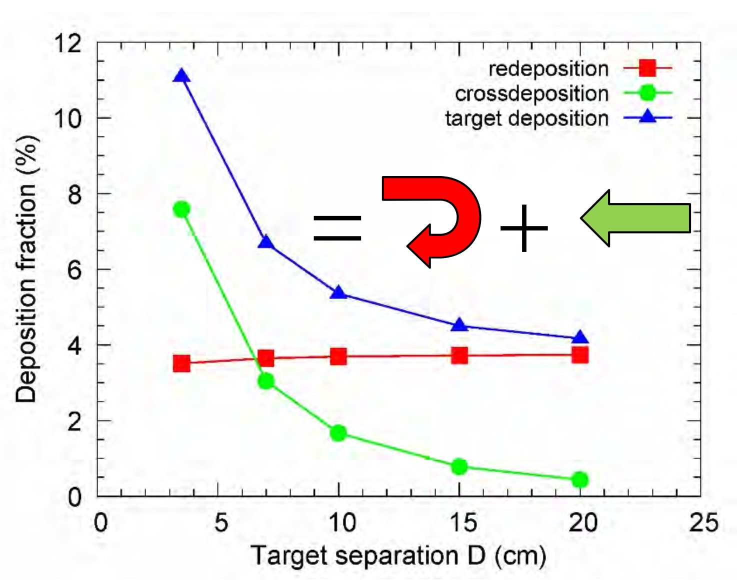
- RSD2013 time solution with redeposition
- Multicell target/substrate with varied SiMTra profiles

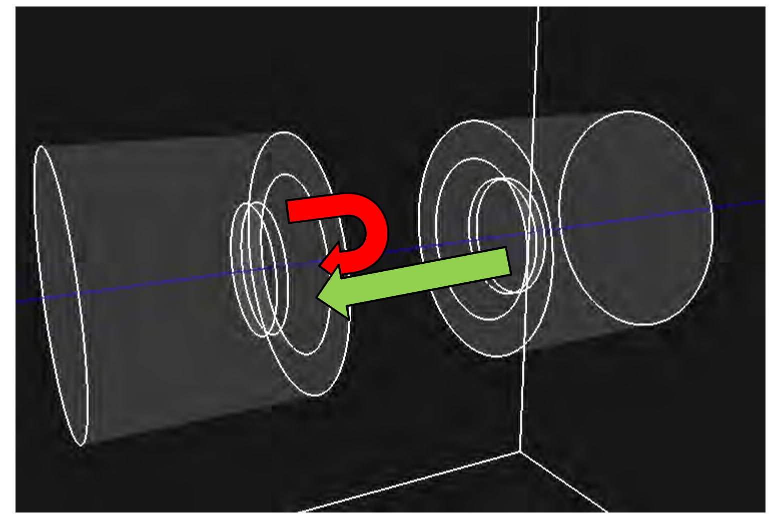






Dual target : target deposition





Decrease 1st critical point is substrate driven:

- Target deposition ↗ substrate deposition ↘
- Target separation ↘ effective substrate area ↘

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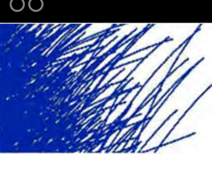
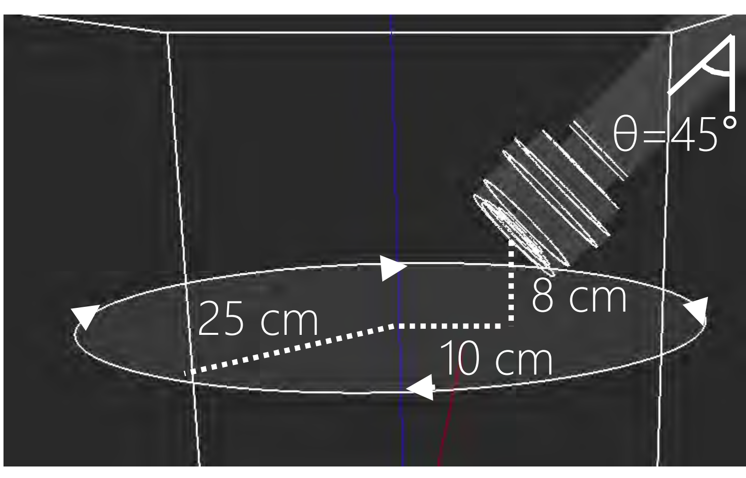
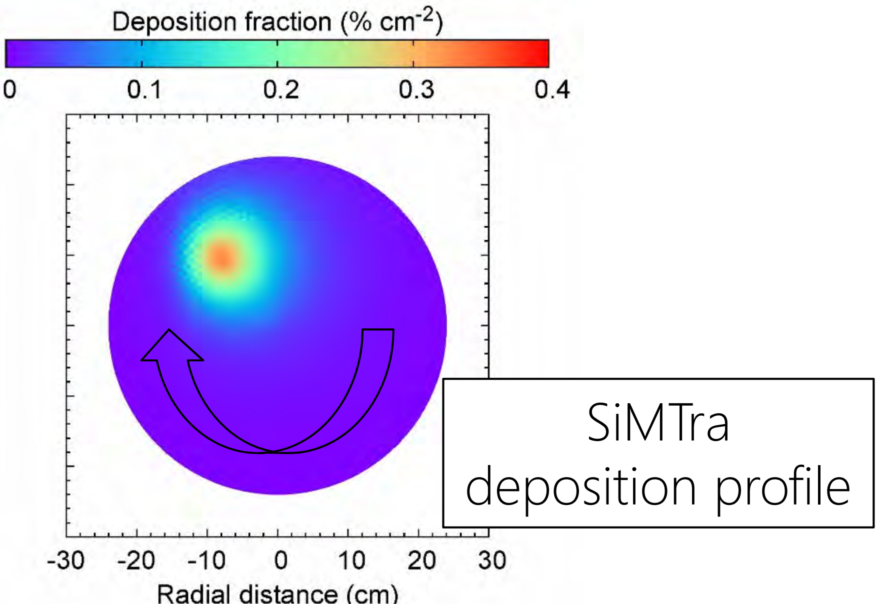


Substrate rotation: experiment

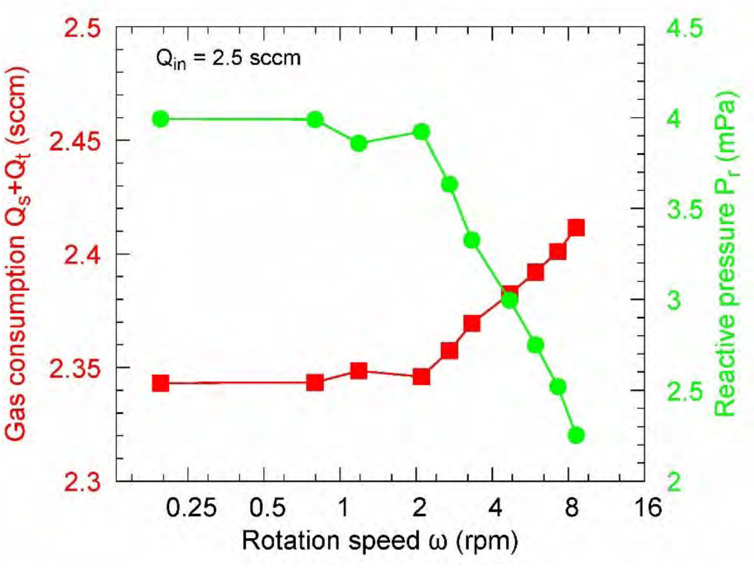




SiMTra deposition profile

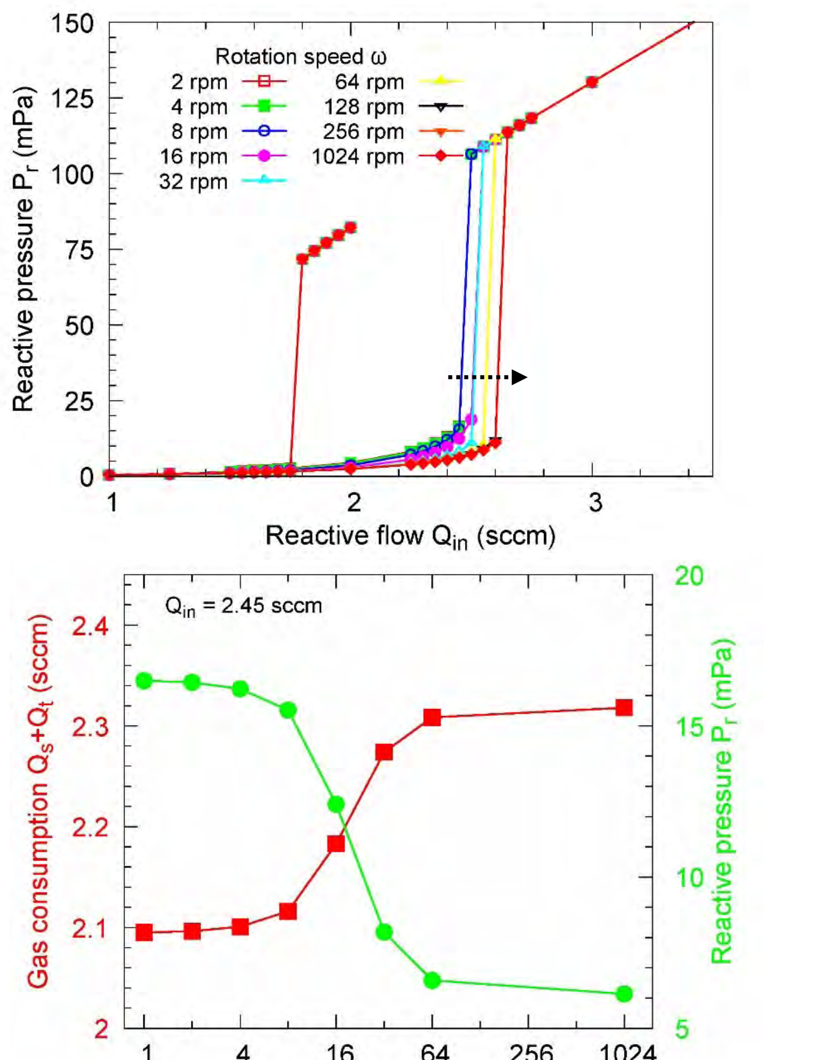
Conditions:

- cuboid chamber (50 x 50 x 50 cm)
- 2″ circular Al target
- gasses Ar (0.4 Pa) / O_2 (2.5 sccm)
- rotating disk
- pumping 40 Ls^{-1}
- discharge current 0.5 A



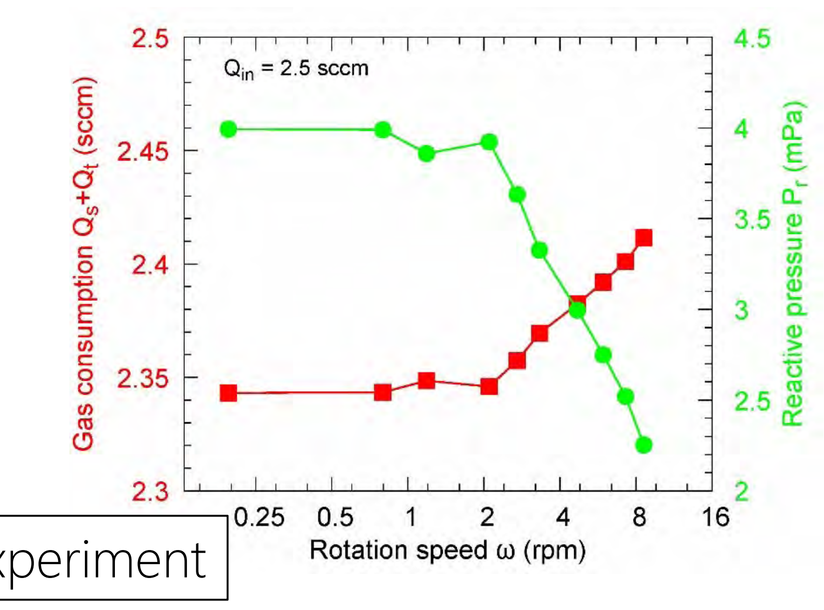
$$Q_s + Q_t = Q_{in} - P_r S$$

Substrate rotation: simulation



Rotation speed on hysteresis:

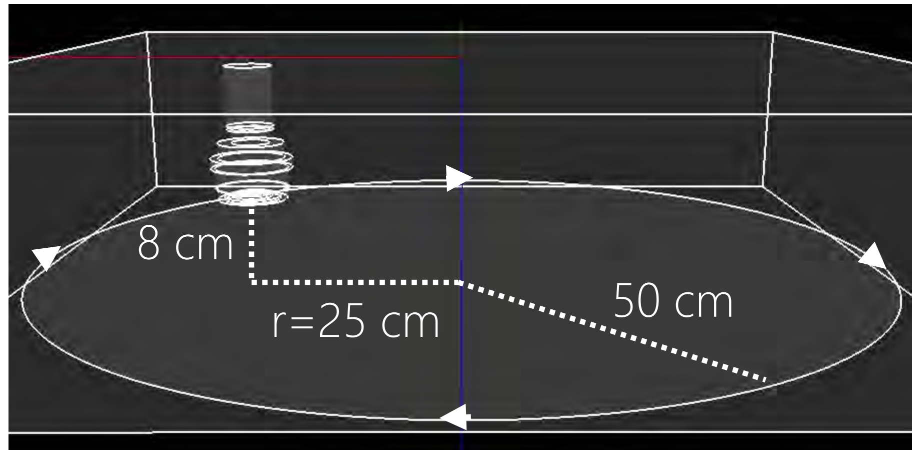
- 1st critical point slightly increases
  - ➢ experimental not resolvable
- enhanced substrate gettering
  - ➢ experimental resolvable
- 2nd critical point unaffected



Simulation

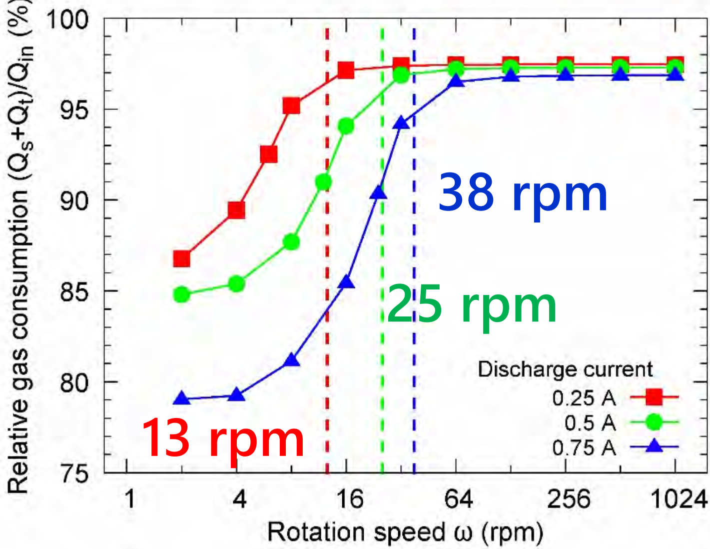
Experiment

Substrate rotation: simulation times two…

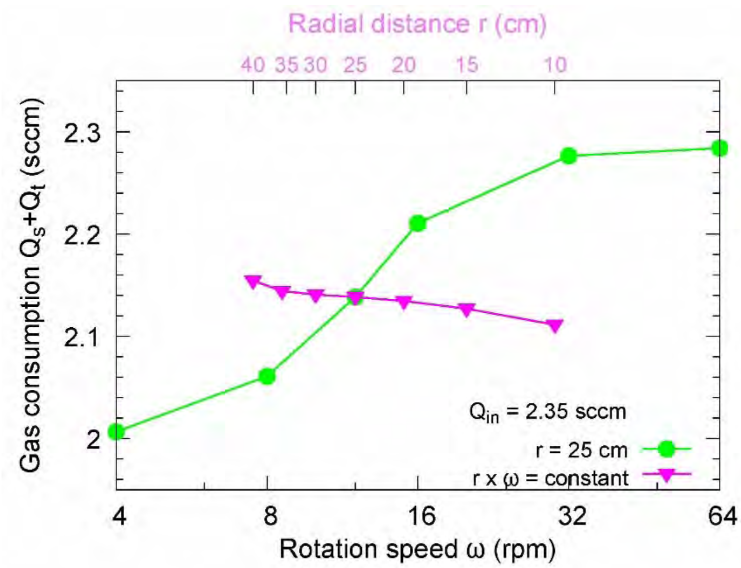


Conditions:

- chamber (100 x 100 x 25 cm)
- 2″ circular Al target (0°)
- gasses Ar (0.4 Pa) / O_2
- rotating disk
- pumping 40 Ls^{-1}
- discharge current 0.5 A

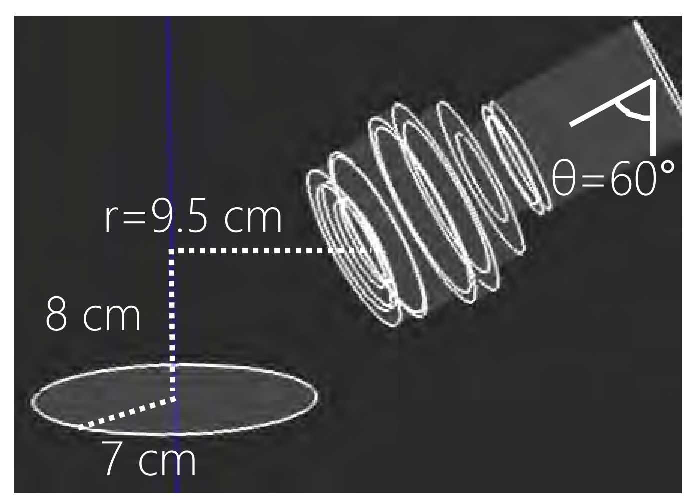


Maximum gas consumption around one monolayer per rotation



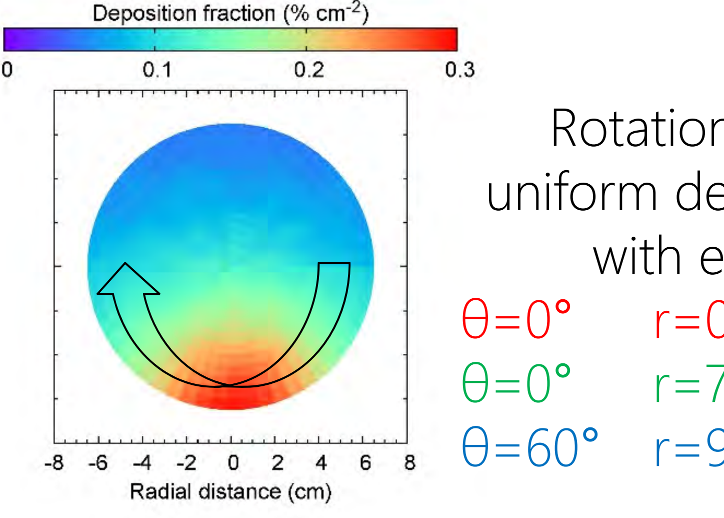
Gas consumption depends on surface speed r x ω

Substrate rotation: uniform thickness



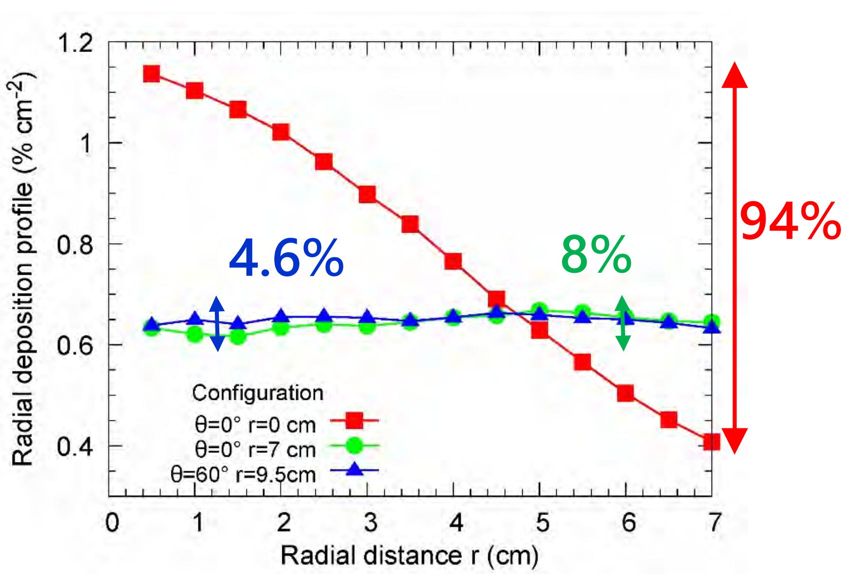
Conditions:

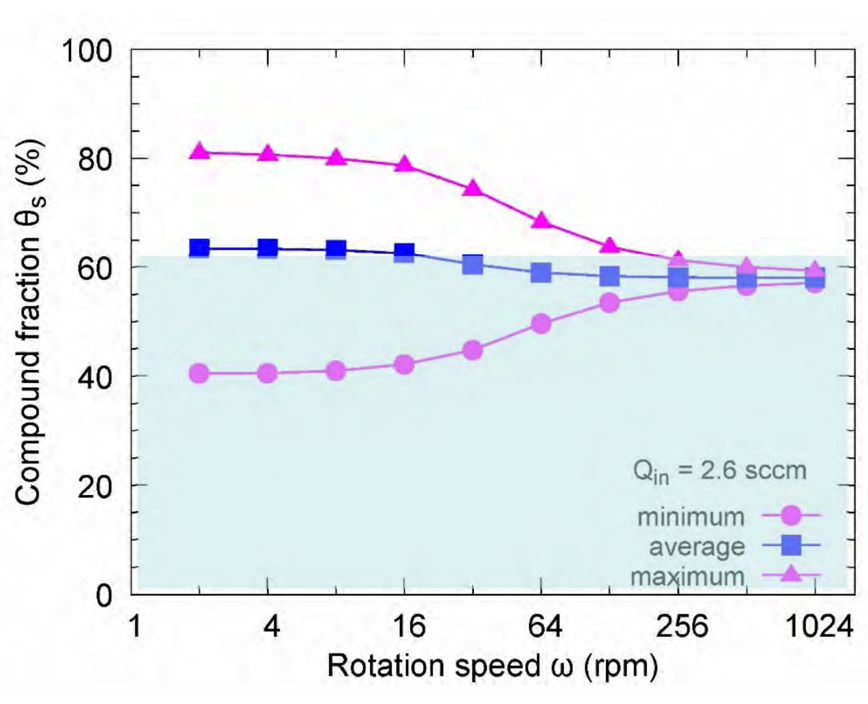
- cuboid chamber (50 x 50 x 50 cm)
- 2″ circular Al target
- gasses Ar (0.4 Pa) / O_2
- rotating disk
- pumping 40 Ls^{-1} and 80 Ls^{-1}
- discharge current 0.5 A and 1 A

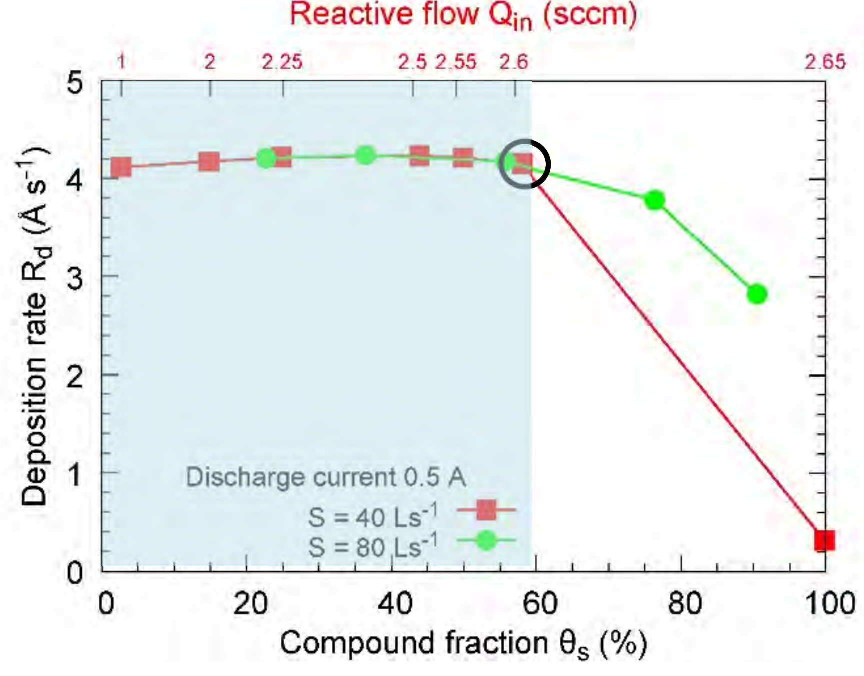


Rotation results in uniform deposition rate with efficiency

θ=0°	r=0cm	**35%**
θ=0°	r=7cm	**21%**
θ=60°	r=9.5cm	**18%**







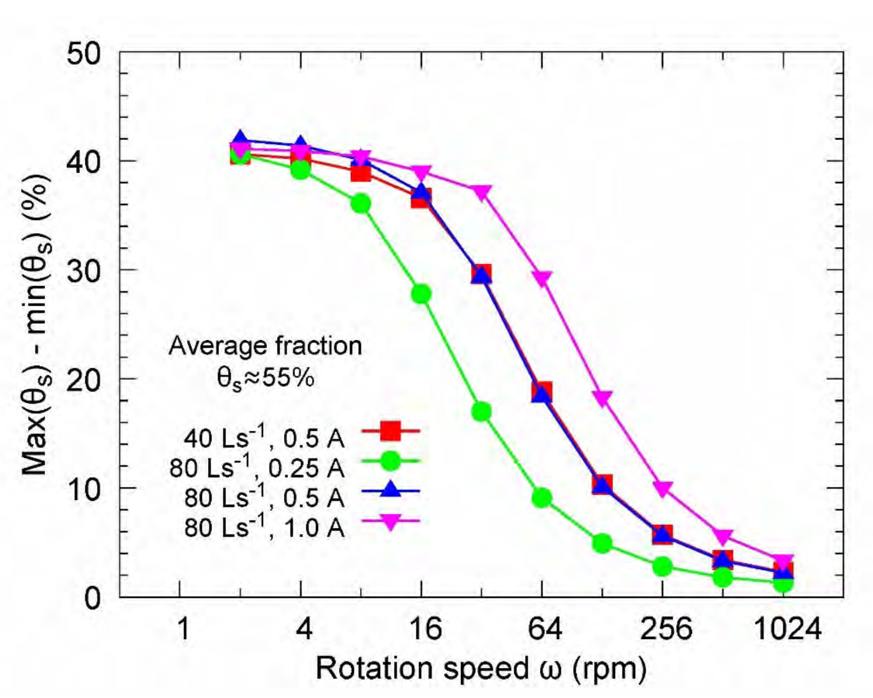
40 Ls^{-1}

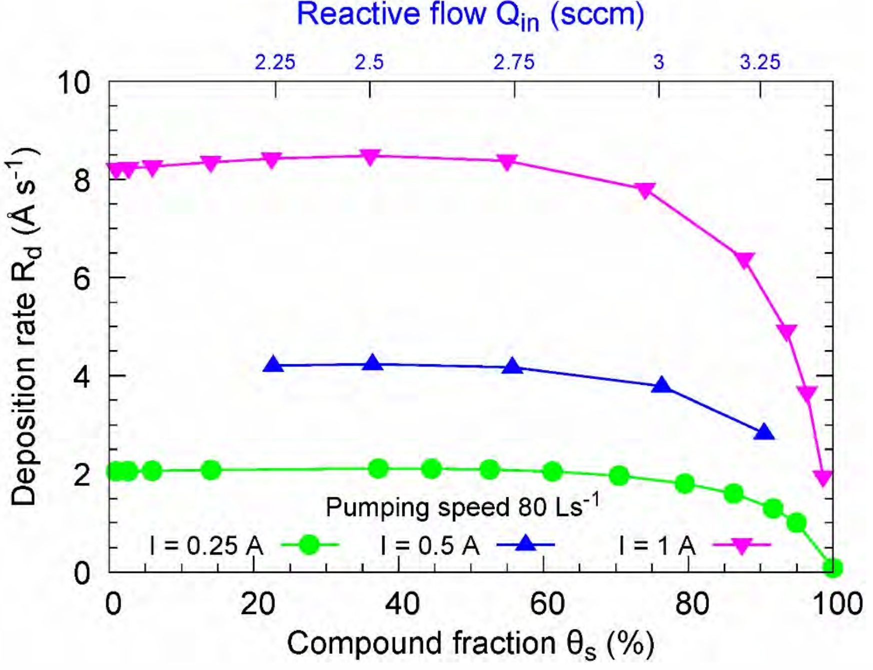
- just before 1st critical point
- rotation speed ↗
  uniformity ↗
- limited fractions (< 60%)

80 Ls^{-1}

- metallic deposition rates
- pumping speed ↗
  range of fraction ↗ (< 95%)

Substrate rotation: tunable deposition rate





Spread in stoichiometry

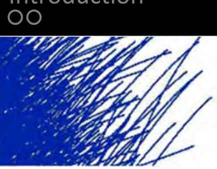
- almost independent of pumping speed
- increases with discharge current

Deposition rate scales with discharge current

Efficiency = high pumping speed, high current and high rotation speed

Conclusion

- The RSD2013 software is a dynamic and **user-friendly** tool to simulate the **hysteresis** during reactive sputtering.
- **Ratio of oxide sputter yields** and **(k, Y_c) correlation** seems highly independent of exact RSD model choice.
- **Redeposition** influences the shape of the racetrack and the sputter profile on the target, which are no synonyms.
- The target separation in a **dual magnetron system** influences the hysteresis.
- A tunable, uniform stoichiometry and film thickness can be obtained by **substrate rotation**.



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At DRAFT we want to become the recognized leader in the understanding of thin film growth by reactive magnetron sputtering
and
to enjoy research by experiments and simulations.

Design, Research And Feasibility of Thin Films