



Virtual Coater™ by fast computer modeling algorithms:

From nano to mm size 3D simulations

S. Lucas,
Innovative Coating Solutions & UNamur

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Current situation

- We all have PVD machines that are expensive
- Access to these machines is limited
- Developing a product is time consuming and expensive
- Product properties are not always well understood
- Coater design takes also times

**Fast and versatile Virtual
Coater**

Virtual Coater™

1. DEFINE

Create your own PVD process by digitizing your deposition machine & substrates geometry in Virtual Coater™.

Types of Coaters



Batch coater



Cluster coater



Inline coater

Source Parameters



Single



vs.



Multiple



Metallic

vs.



Reactive

Substrates Parameters



CAD



Fixture



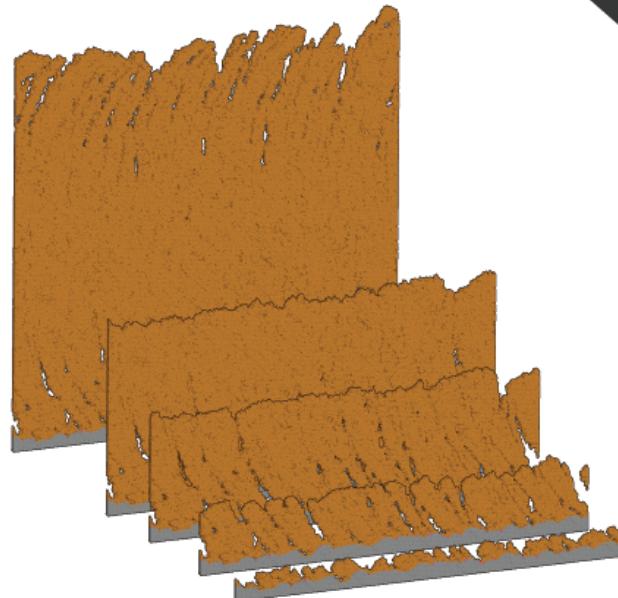
Linear Motion Multiple Rotations

2. SIMULATE

Virtual Coater™ uses NASCAM*, a powerful film growth modeling module developed by ICS.

*NANoSCale Modeling Code that uses kinetic Monte-Carlo simulation.

It is the **fastest** & most **detailed** simulating tool of film growth on your substrates.



3. ANALYZE

Virtual Coater™ analyses the properties of your coated substrates.



Film Growth



Electrical Properties



Optical & Color Properties



Elastic Properties



Thermal Properties



Surface Roughness



Porosity & Pore Detection Visualization



And much more!

Virtual Coater: fast algorithms & easy to use (800 lic.)



Virtual Coater V4.8.2

File Run Window Examples Tools Help

optical_coating x

Make Process - V3.1 - 30/03/23

Parameters Results Log Stacks

Parameter Tables

ID	Type	R	θ	Z	ϕ	ψ	On
1	Magnetron	0.3	0	0	180	0	<input checked="" type="checkbox"/>
2	Magnetron	0.3	120	0	180	0	<input checked="" type="checkbox"/>
3	Magnetron	0.3	240	0	180	0	<input checked="" type="checkbox"/>

Generate Project

16.7 cm

top

s1 s2

racetrack_profile

General Parameters

Stack name : mp

Time unit : minutes

16/200 Reload

Graph

final_composition... Open Reload Close Simulation Results

level_No

Transmittance(%): Si Ti O Ar Xx Ag Cu

Optics

RTA - Transmittance - unpol.csv - Transmittance:unpolarized-light

Transmittance:unpolarized-light

wavelength(nm)

0.00deg. 7.73deg. 15.45deg. 23.18deg. 30.91deg.

38.64deg. 46.36deg. 54.09deg. 61.82deg. 69.55deg.

77.27deg. 85.00deg.

Jmol

film_g... Open Reload Close Simulation Results

Results Parameters Log Image

racetrack_profile

File Collection of 94 mod... model 94/94 Configurations

Select (8012128) View Style Color Surfaces Symmetry Scenes Zoom Spin Vibration Spectra Animation

Measurements Set picking Console JavaScript Console Show Computation Language About...

Play Pause Resume Stop Next Frame Previous Frame Rewind Reverse Restart Set FPS

Porosity

Jmol - Pores - All kind.xyz

Jmol

The screenshot displays the Virtual Coater software interface, version V4.8.2. The main window is titled 'optical_coating' and shows several panels: 'Make Process' (V3.1 - 30/03/23), 'Graph' (final_composition...), 'Optics' (RTA - Transmittance - unpol.csv - Transmittance:unpolarized-light), and 'Porosity' (Jmol - Pores - All kind.xyz). The 'Make Process' panel includes tabs for 'Parameters', 'Results', 'Log', and 'Stacks', and contains a 'Parameter Tables' section with three Magnetron sources. The 'Graph' panel shows transmittance levels for various elements across a wavelength range from 200 to 1,000 nm. The 'Optics' panel displays a plot of transmittance versus wavelength. The 'Porosity' panel shows a 3D visualization of a porous film structure with a color-coded porosity map. A context menu is open over the 3D visualization, providing options for file operations, selection, style, surfaces, scenes, and animation controls. The 'Animation' section of the menu is expanded, showing options like Play, Pause, Resume, Stop, and various frame navigation controls.

Virtual Coater

- « 2D substrates »: validated

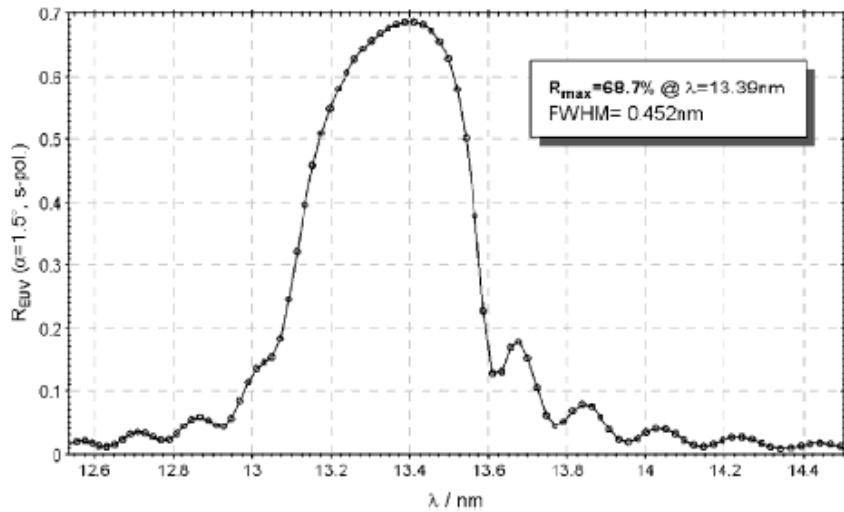


Figure 44: EUV reflectivity of pure Mo/Si-multilayers (dperiod = 6.82 nm, $\alpha = d\text{Mo}/d\text{period} = 0.39$, number of periods N = 65) prepared by MSD (Figure 1 in ref. 4).

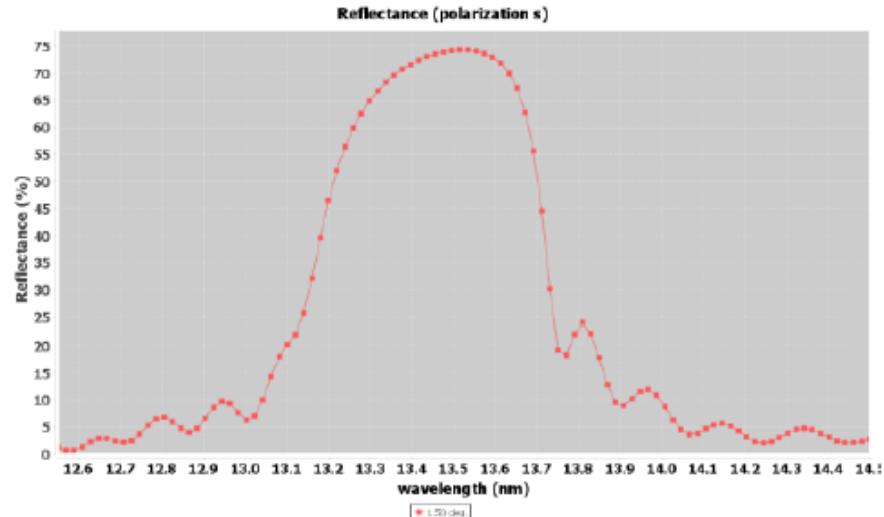
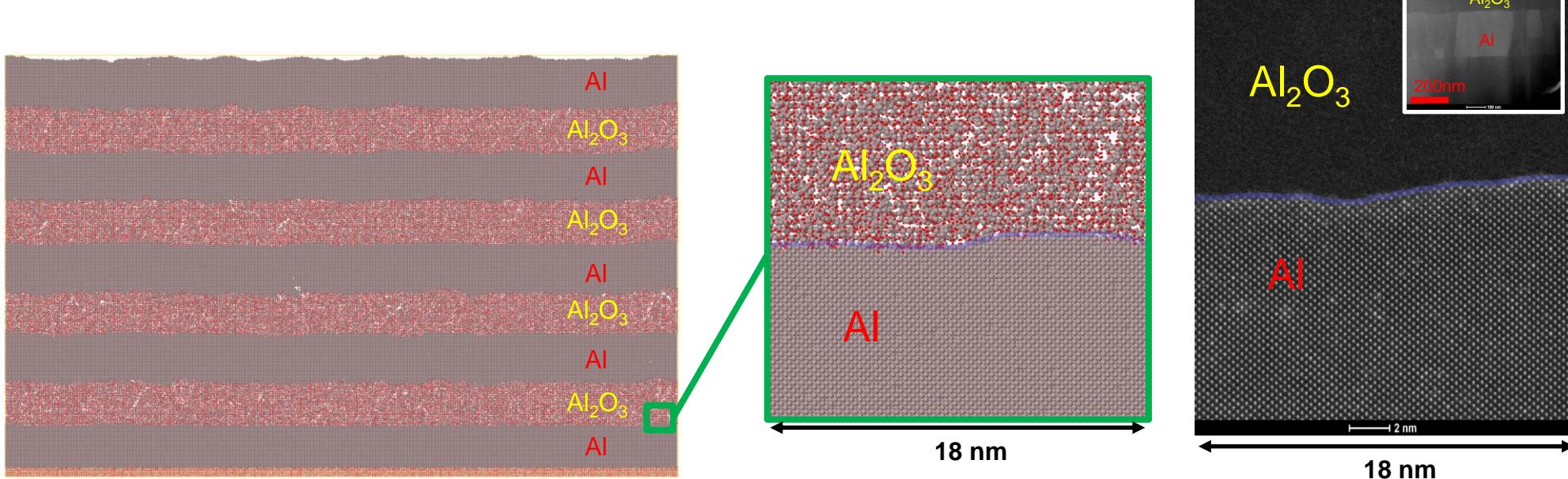
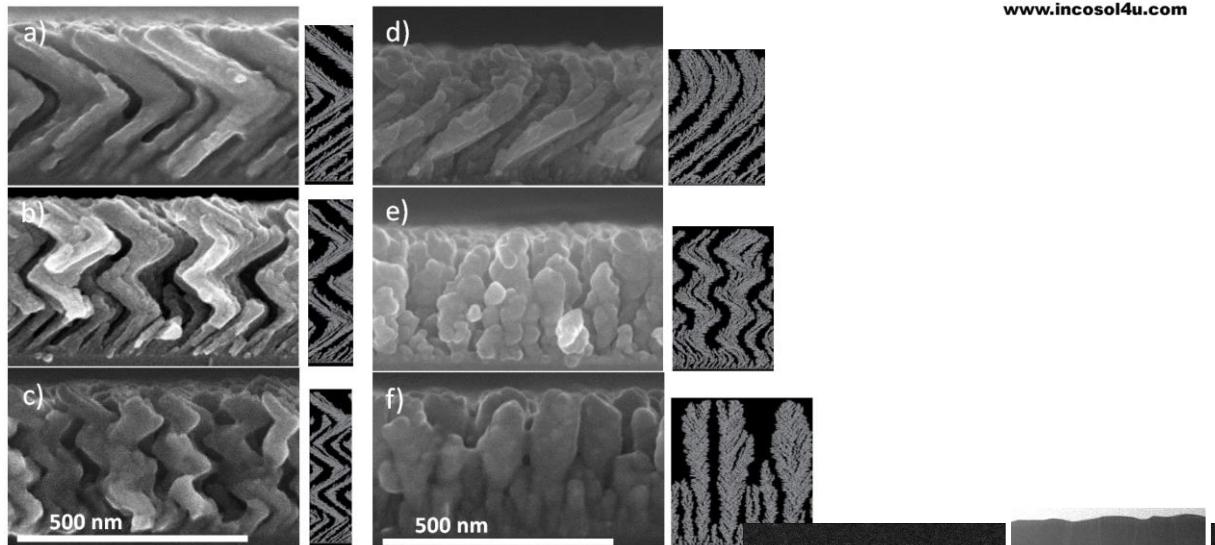


Figure 45: EUV reflectivity of simulated deposition of Mo/Si-multilayers and computed by the *Optics* plugin.

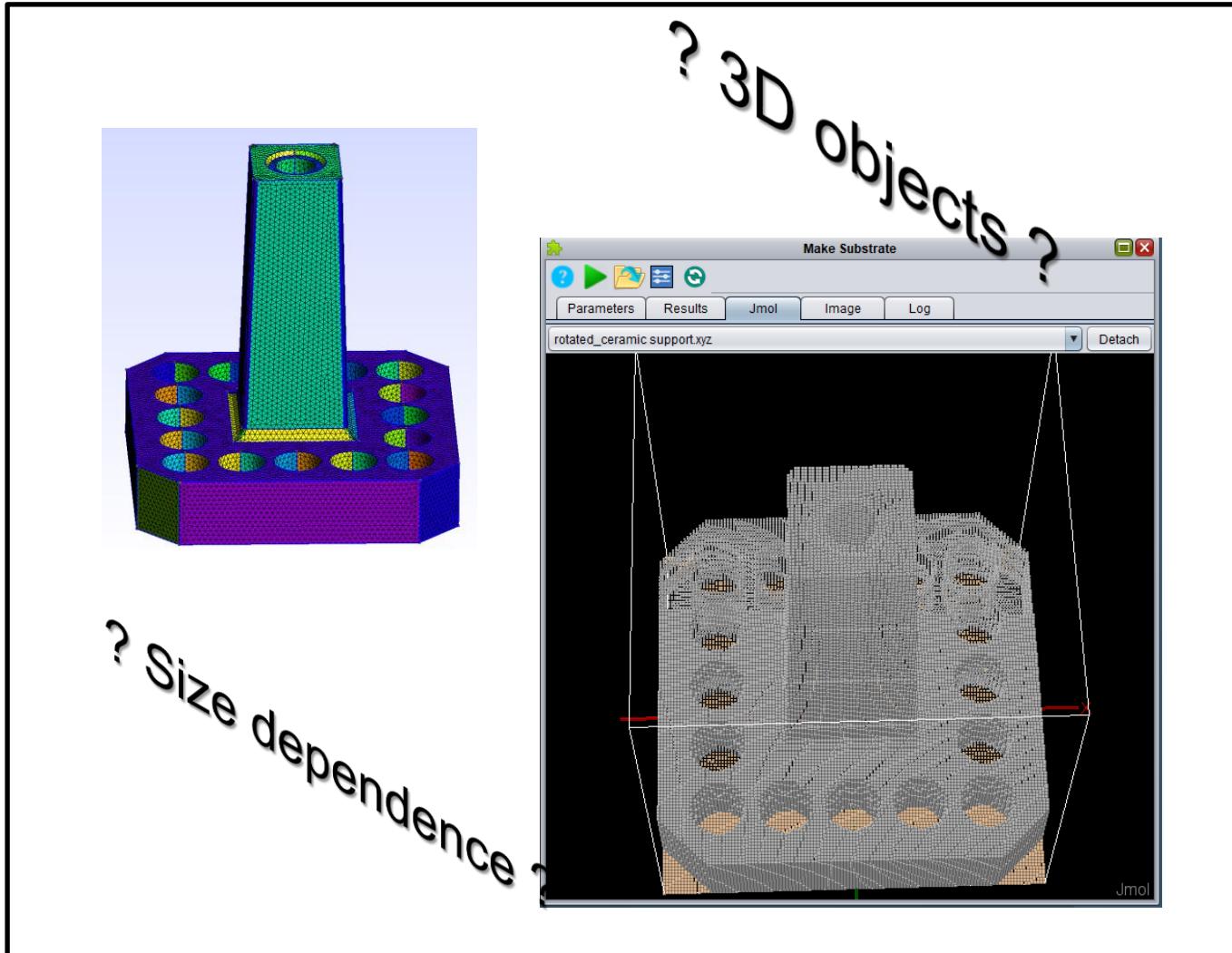
Virtual Coater

- « 2D substrates »



Virtual Coater

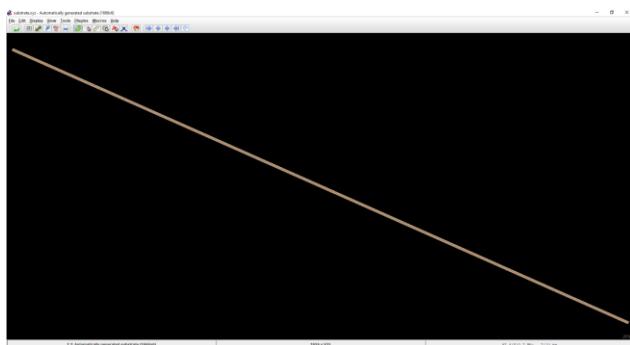
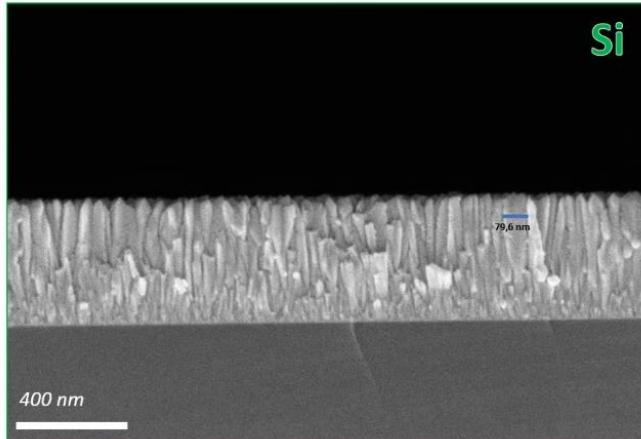
- What about 3D substrates ?



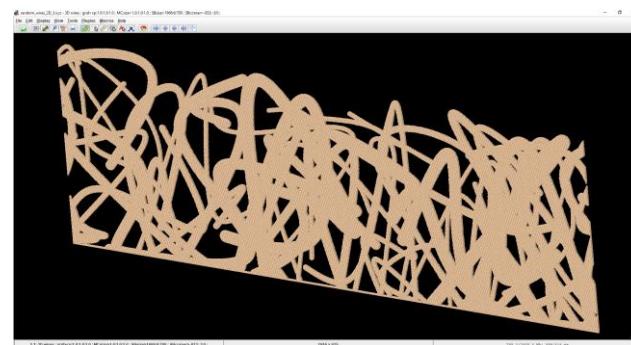
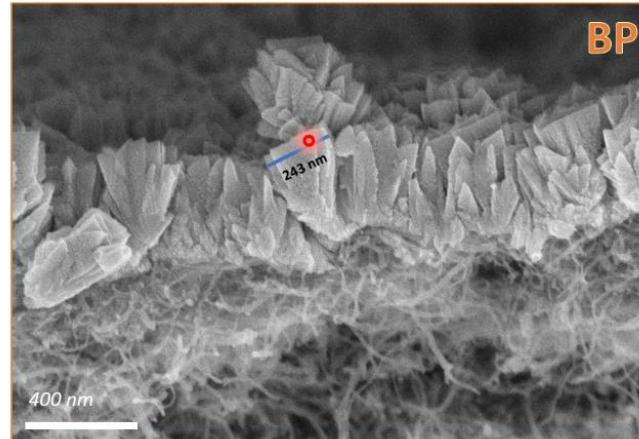
Reactive magnetron sputtering dep. on buckypaper

Studied Substrates:

- Comparison flat substrate VS buckypaper
- 3D simulations ($500\text{nm} \times 3\text{nm} \times 400\text{nm}$)
- Scale: 1:1 (1 atom = 0.2 nm)



Si flat substrate

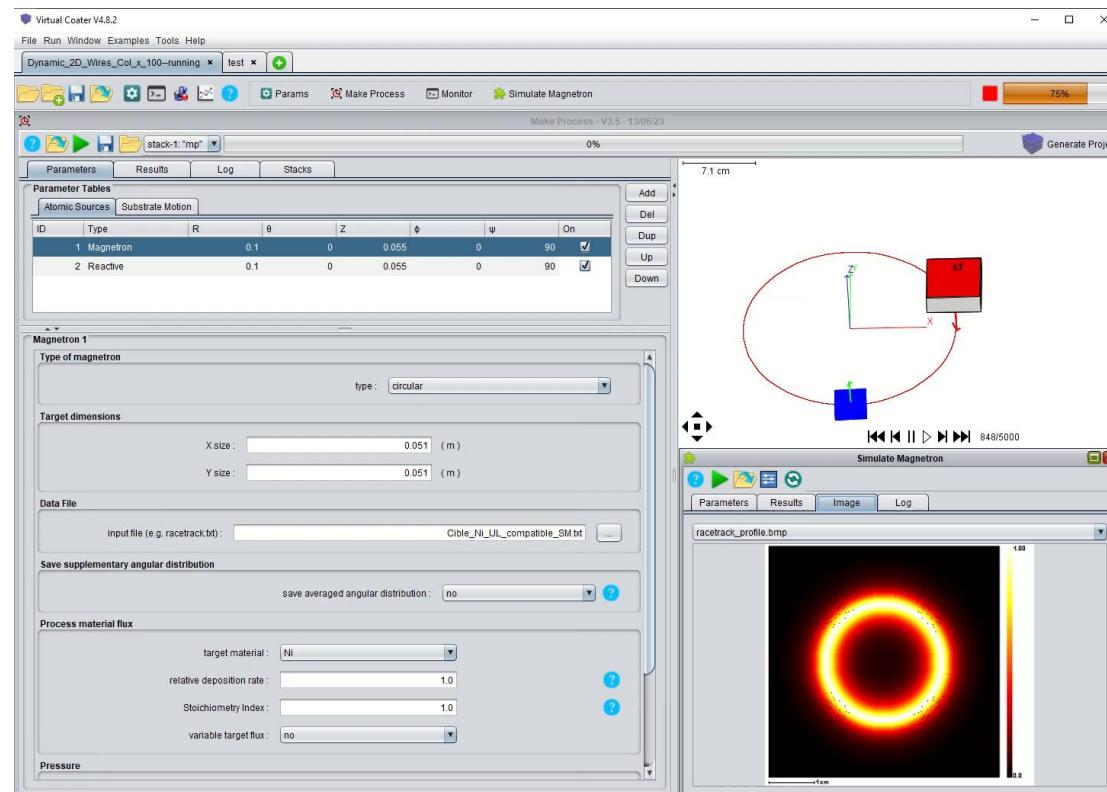
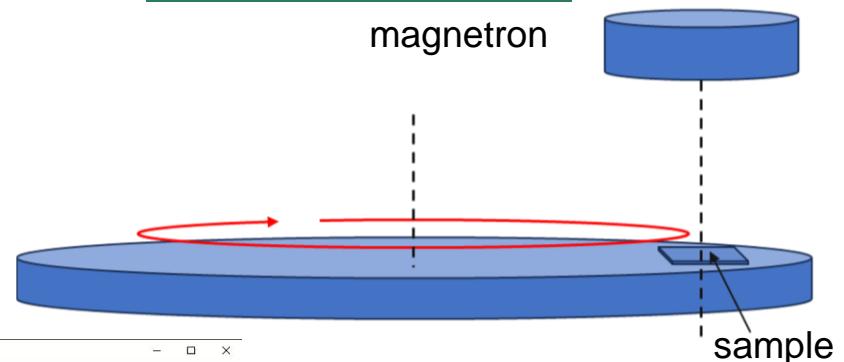
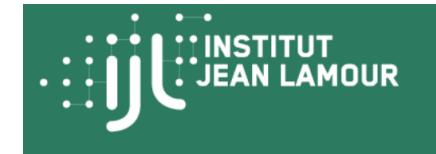


C Buckypaper substrate

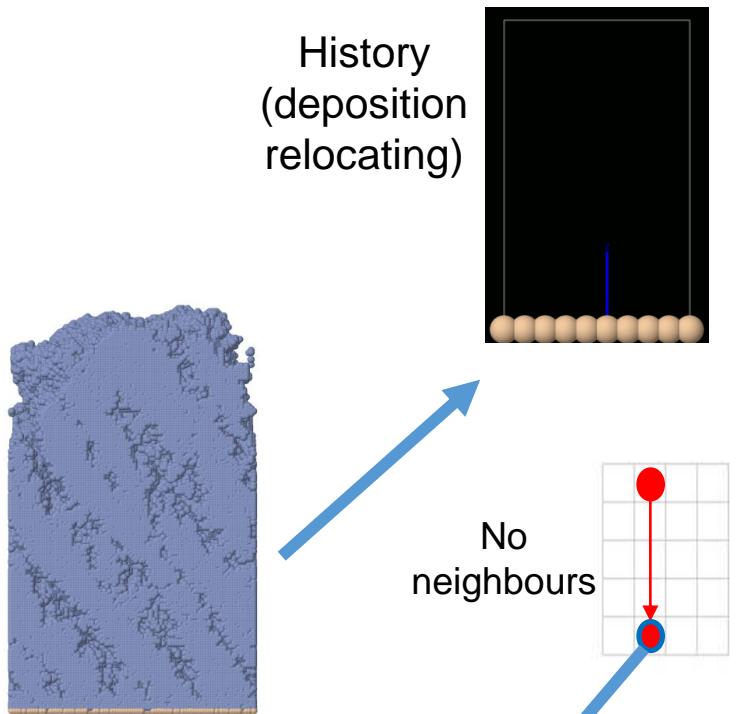
Reactive magnetron sputtering dep. on buckypaper

Deposition process:

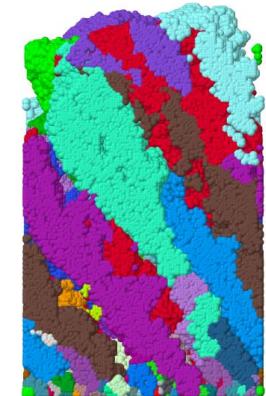
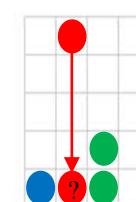
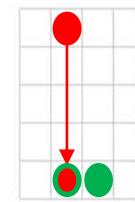
- MeN deposition by RSD
- rotation of the sample (>3000 loops)



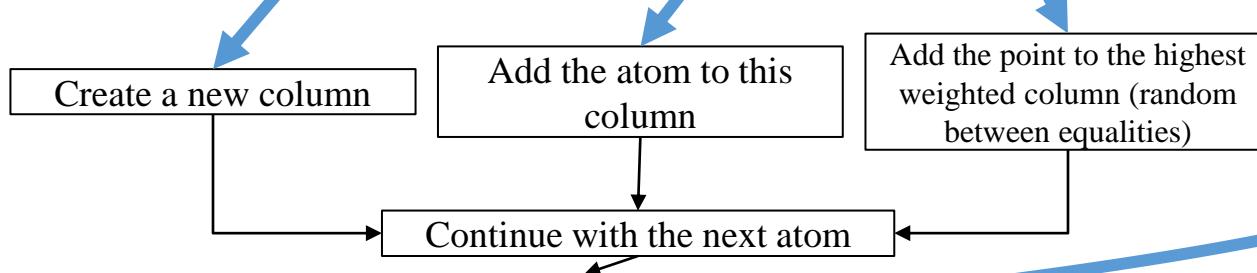
How to visualize Columns ?



Based on the nearest neighbors (deterministic method)



Virtual Coater simulation of a Me film

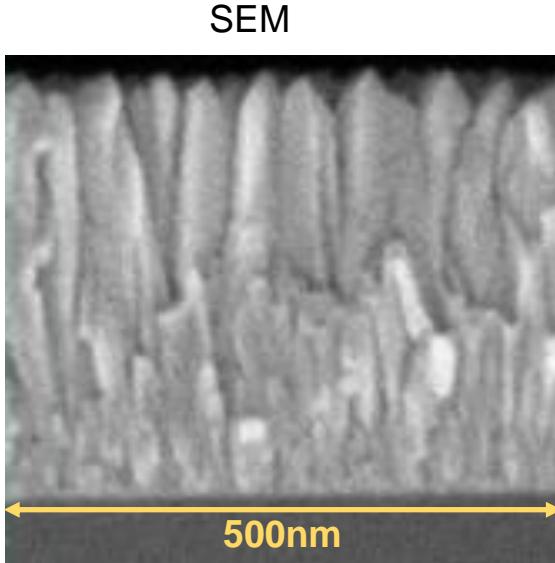


Aurélien Besnard / Noé Watiez

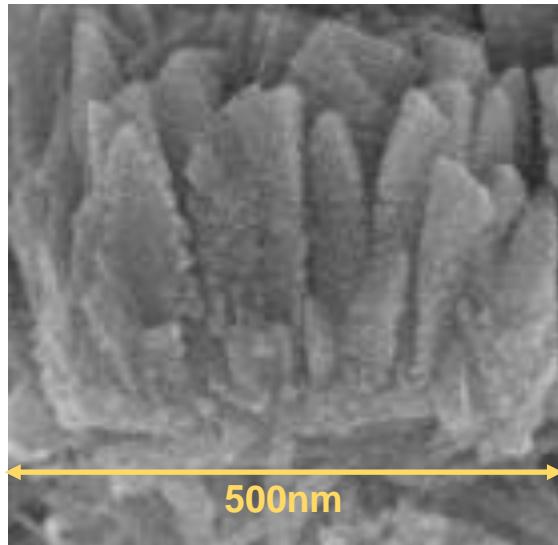
Reactive magnetron sputtering dep. on bucky

Film growth and column detection:

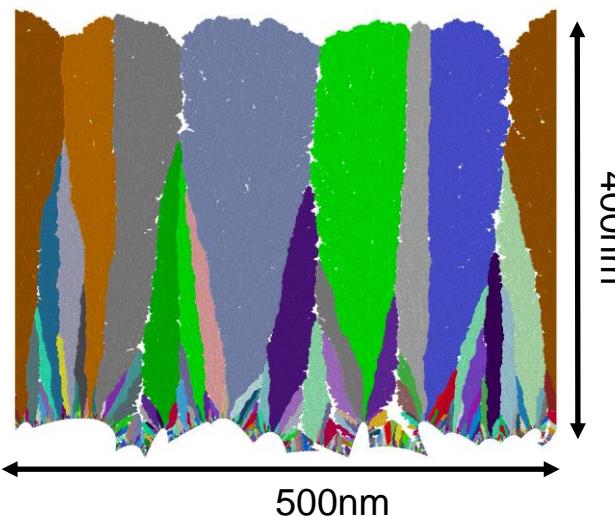
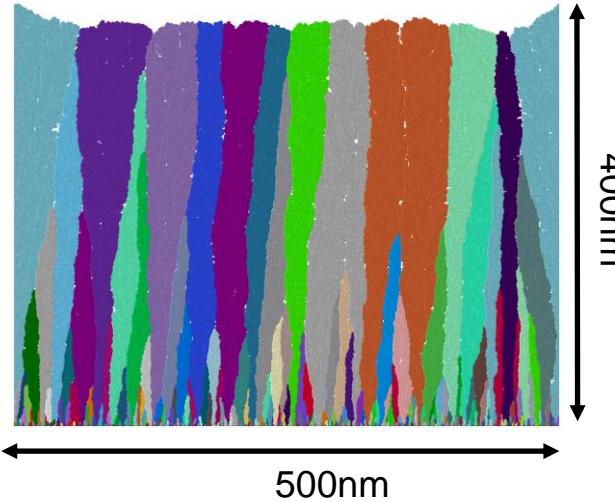
flat substrate



buckypaper



Virtual Coater



Study of the influence of the pressure and rotational motion of 3D substrates processed by magnetron sputtering: A comparative study between Monte Carlo modelling and experiments

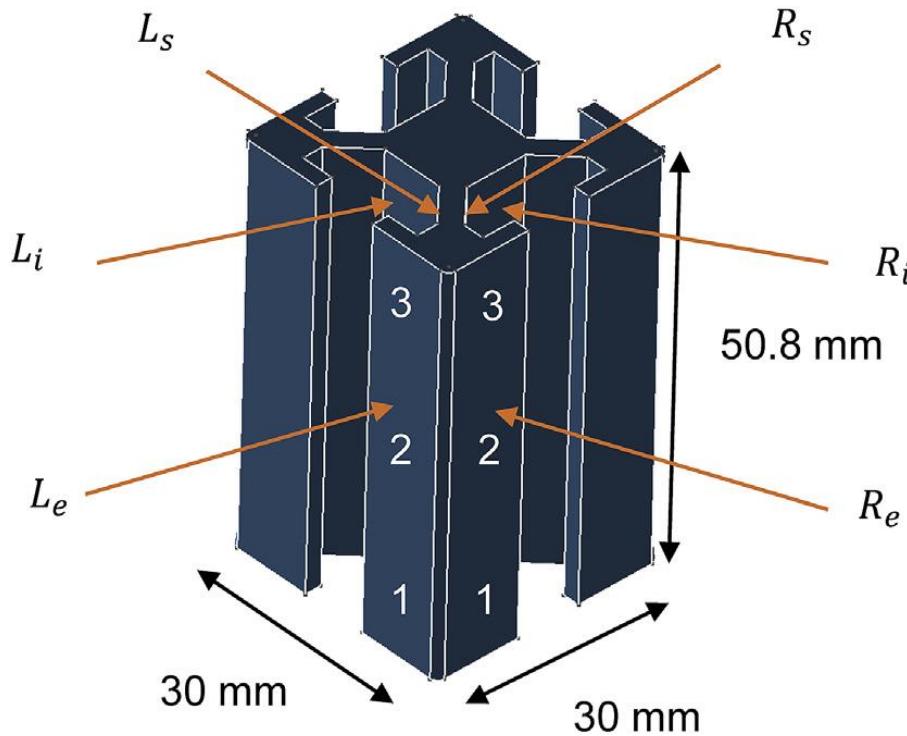
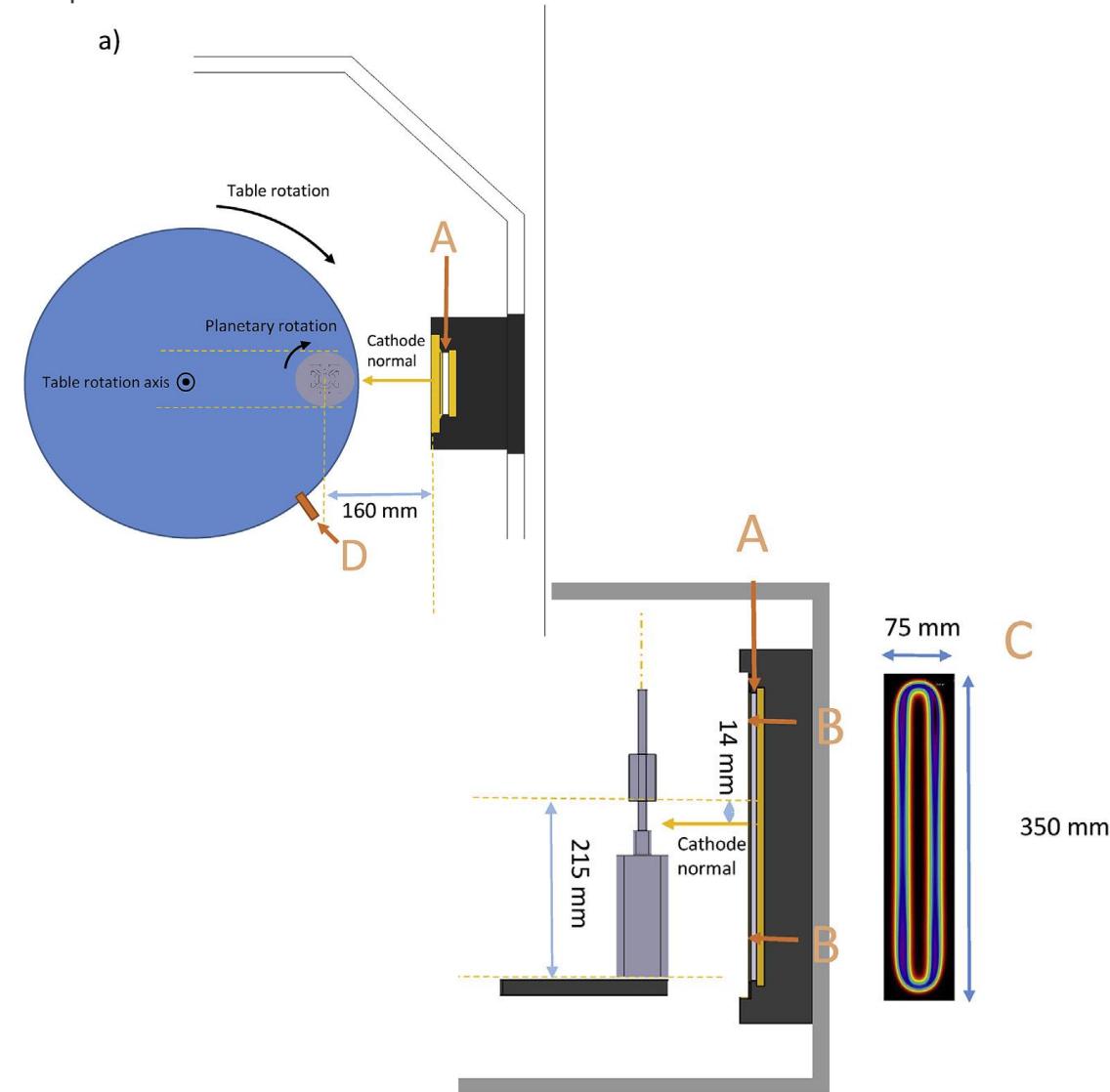


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^b Arts et Metiers ParisTech, LaBoMaP, Rue porte de Paris, F-71250, Cluny, France

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Study of the influence of the pressure and rotational motion of 3D substrates processed by magnetron sputtering: A comparative study between Monte Carlo modelling and experiments



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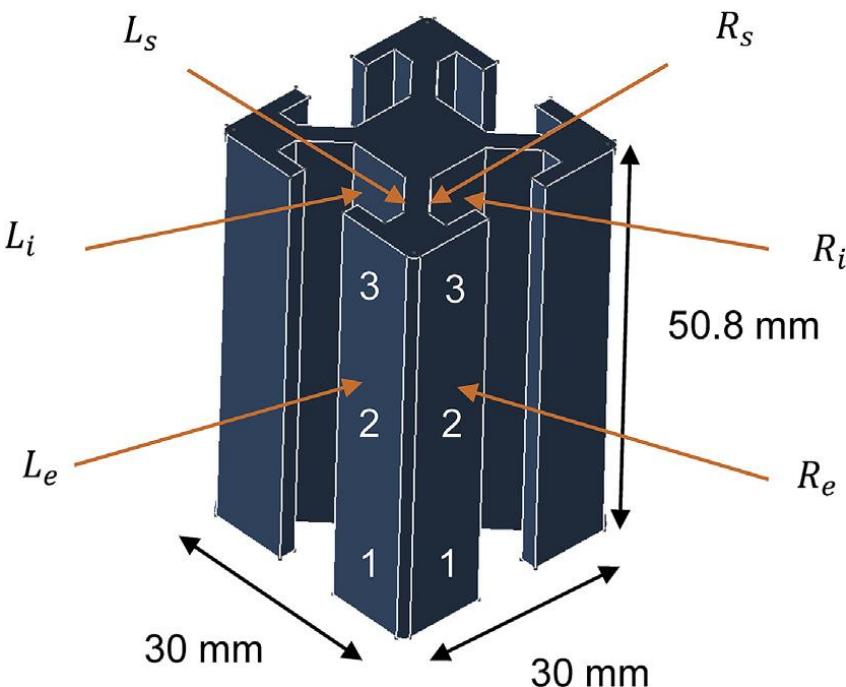
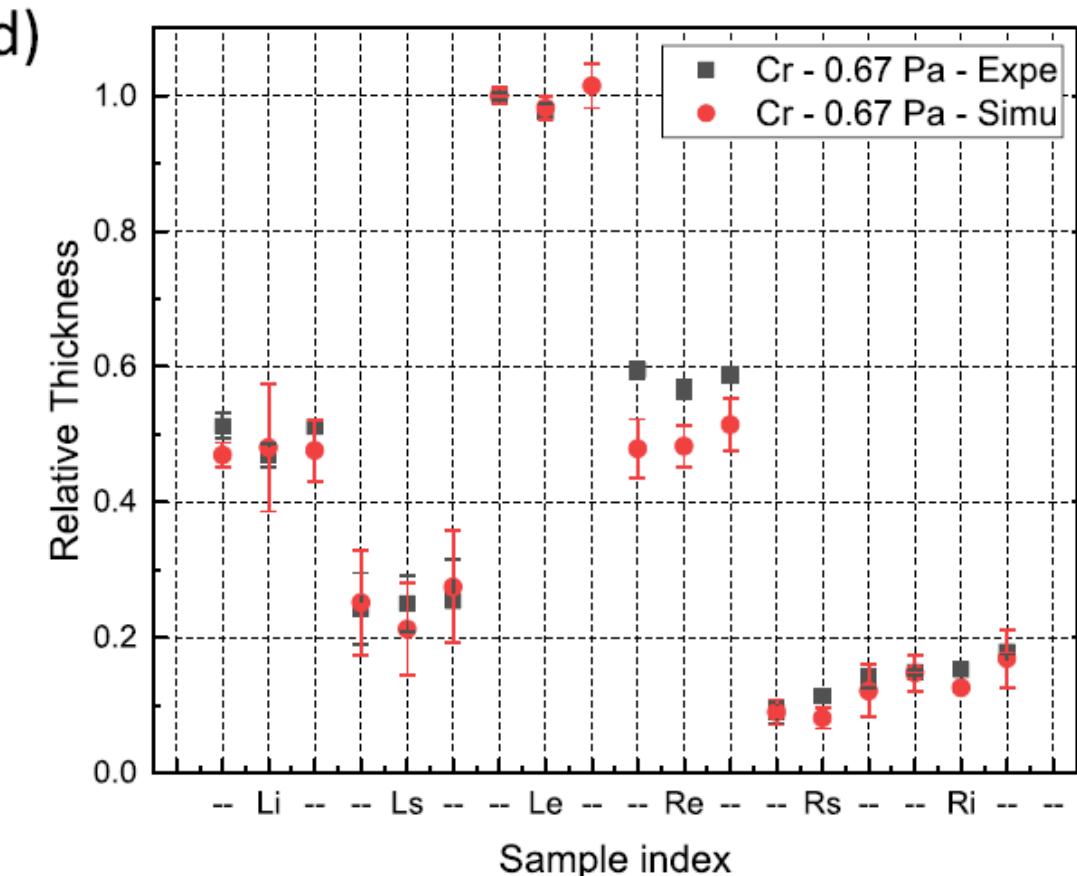


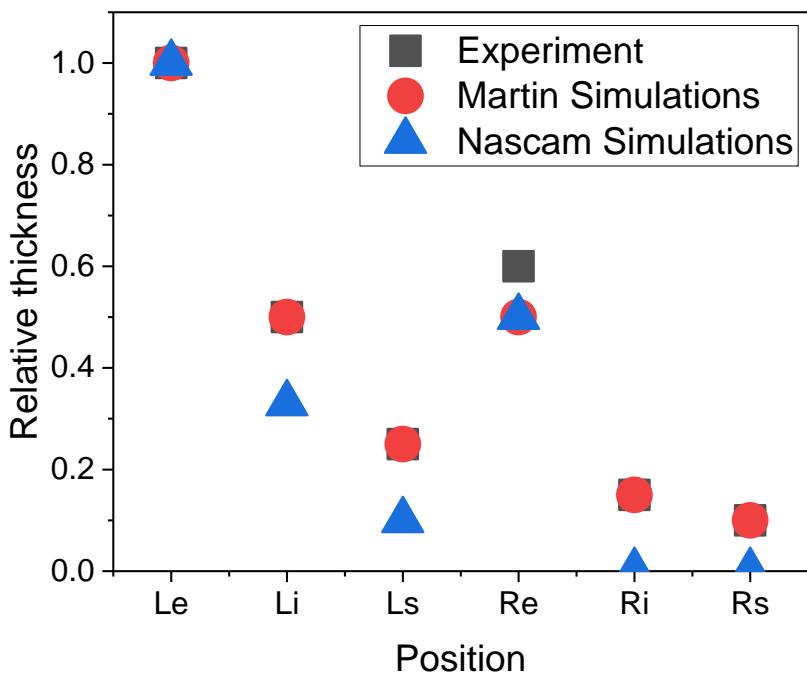
Fig. 4. Meshing of substrate and space cellularisation.



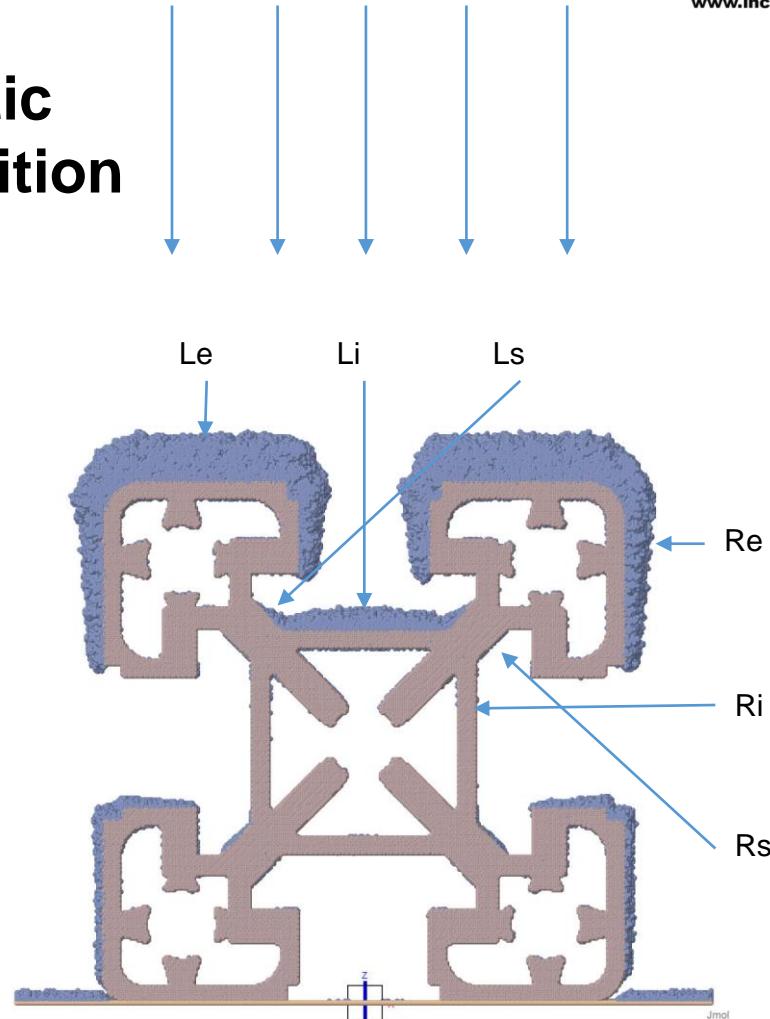
Deposition on 3D mm sized parts

Target : Cr target, dimensions 35 x 7 cm
Pressure : 0.67 Pa (5 mTorr)
Target-substrate distance : 16 cm
Trajectory : **Static position**
Number of magnetrons : 1

300x300x400: 1 atom = 100 μm



Static deposition



Deposition on 3D mm sized parts

1-fold rotation deposition

Target : Cr target, dimensions 35 x 7 cm

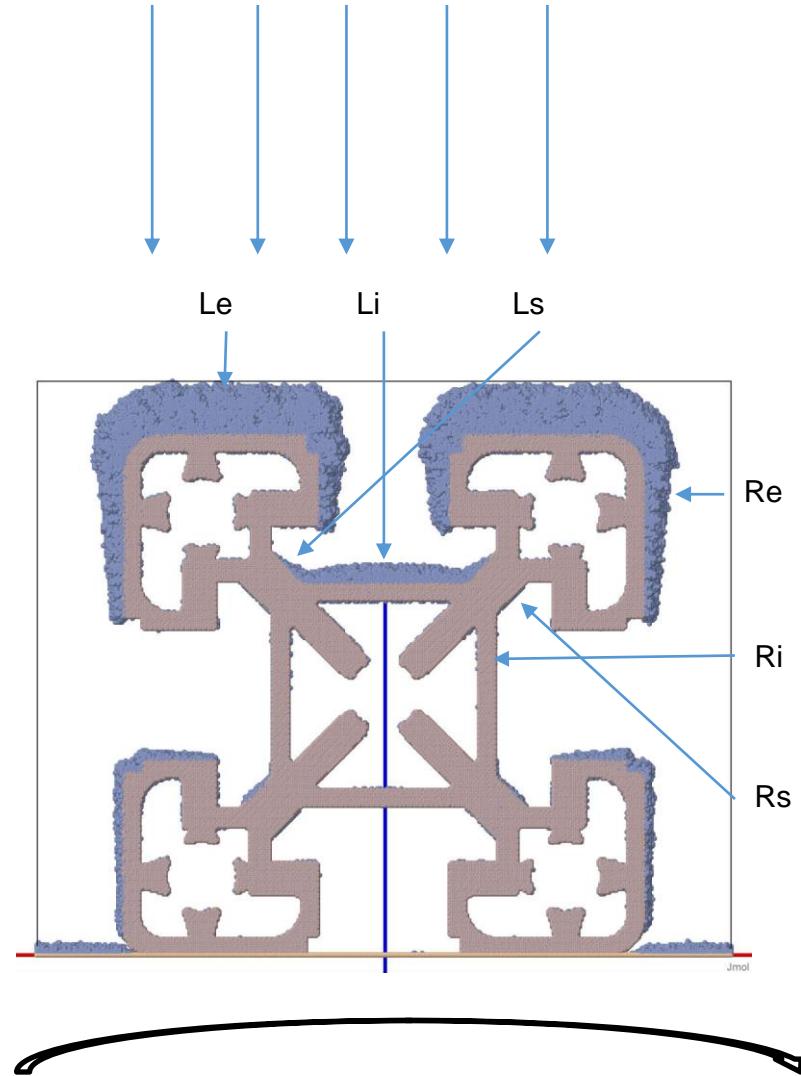
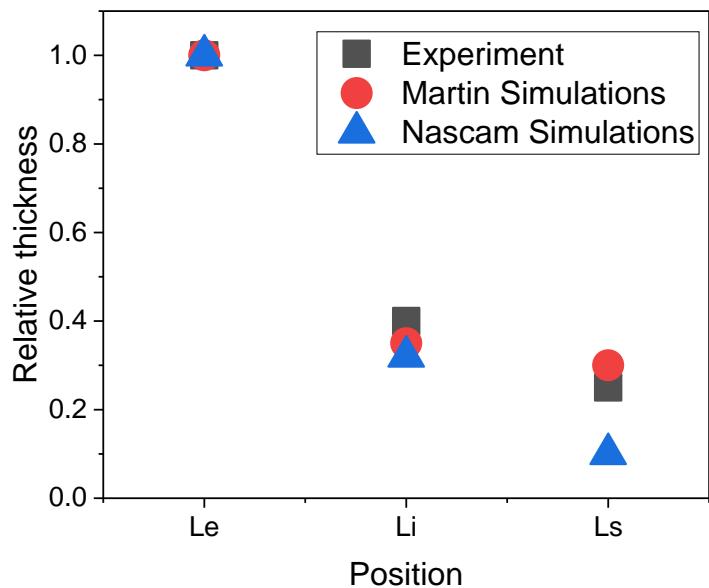
Pressure : 0.67 Pa (5 mTorr)

Target-substrate distance : 16 cm

Trajectory : 1-fold rotation

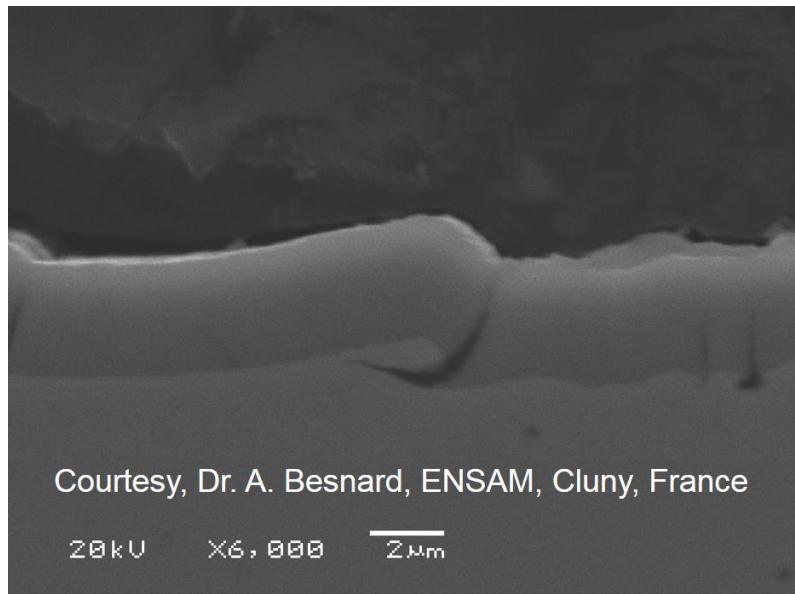
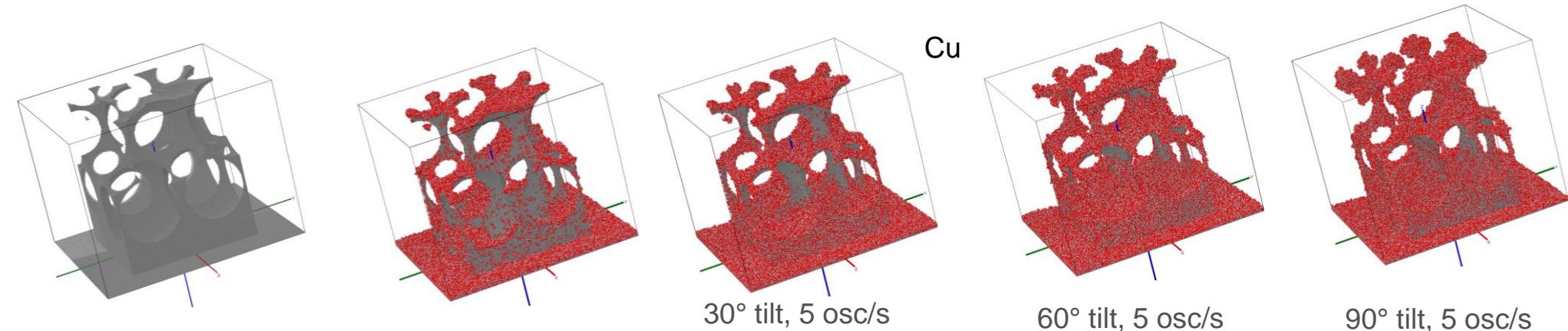
Number of magnetrons : 1

300x300x400: 1 atom = 100 µm

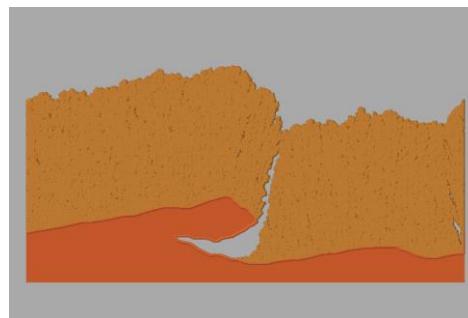


Other cases

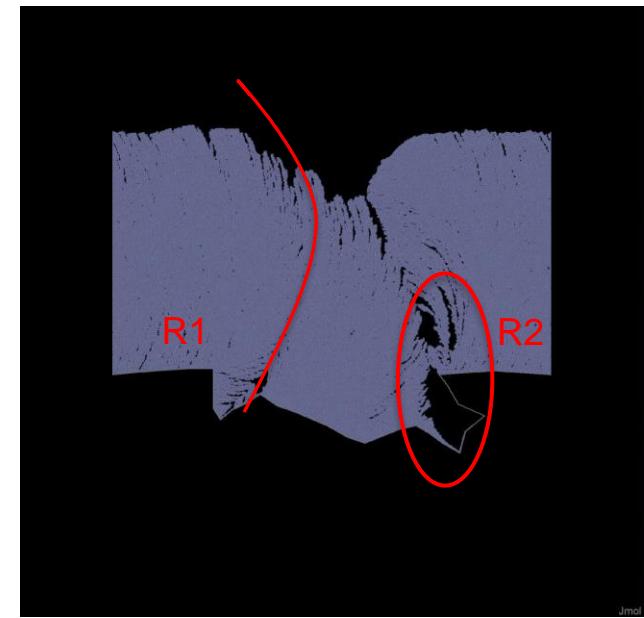
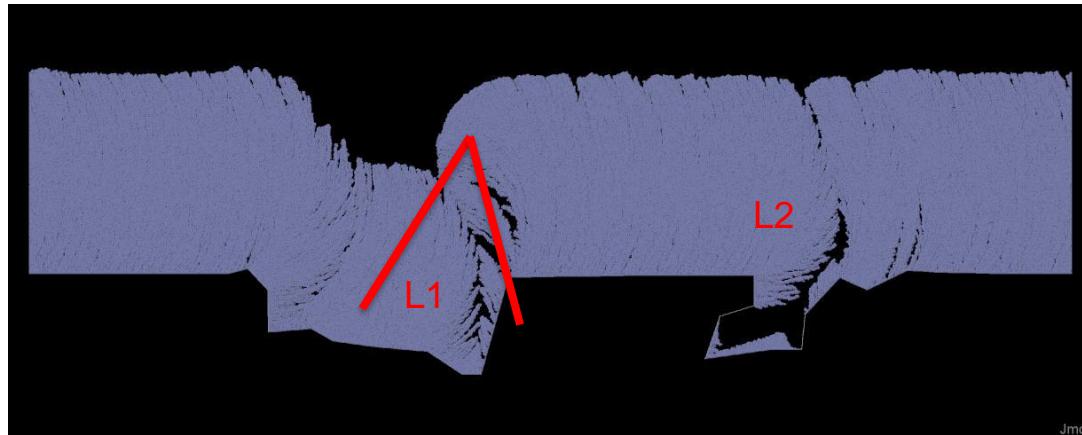
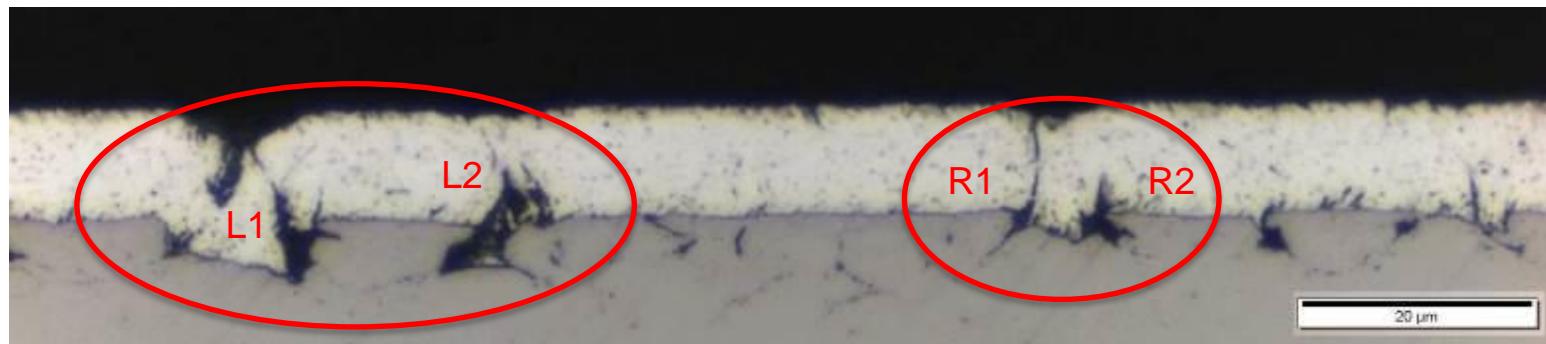
Real foam : 2.5mm ; 1 atom \approx 10 μm



465 atoms : 12 μm / 1 atom \approx 40 μm



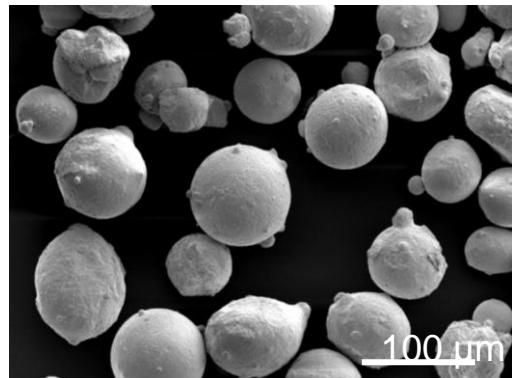
Other cases



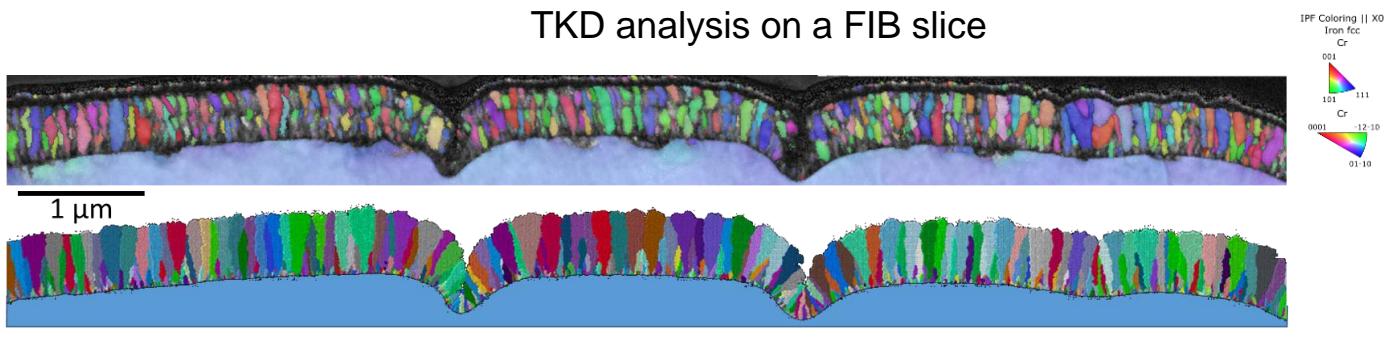
We helped the customer to understand the following:

- What is the effect of the moving strip speed and the deposition rate ?
- What is the effect of pressure ?
- What is the effect of strip temperature ?
- What is the effect of source divergence ?

Other case



Cr deposited on 316L particles



1 at = 4 nm

/!\ the colors only represent columns...
not orientations.

Courtesy Prof. A. Besnard, ENSAM, Fr

Summary

- We all have PVD machines that are expensive with a limited access.
- Easy to use and **FAST** PVD virtual coater is a nice to have
- Our Virtual Coater is fast because it includes fast algorithms related to gas phase calculation and film growth.
- It reproduces very well film growth in several circumstances (coating configuration and process) with the following assumption:
 Properties = f(material deposited / energy and angular distribution / substrate temperature & morphology)
- **Here, we add: our atomistic simulation method can produce realistic simulations on a scale of 1E6 whether it is 1D, 2D or 3D. !**

<u>Case</u>	<u>1 atom ≈</u>
Bucky paper	$2 \times 10^{-4} \mu\text{m}$
Zn defects on Steel	1 μm
Foam	10 μm
Cu defects on Steel	40 μm
Metallic profile	100 μm

- **The only main limitation know today is hidden surface facing the incident direction**

Many Thanks

slu@incosol4u.com / www.incosol4u.com



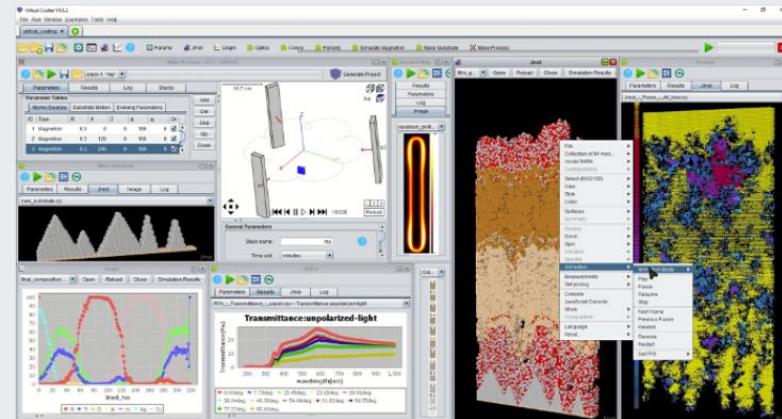
Modeling and simulation

Do you want to outsource modeling or buy a state of the art film growth simulation software ?



Service

We provide services in simulation of coating deposition by PVD



Software sales

ICS is the exclusive dealer of Virtual Coater simulation suite