INNOVATIVE COATING SOLUTIONS

Virtual Coater^{TM} by fast computer modeling algorithms:

From nano to mm size 3D simulations

S. Lucas,

Innovative Coating Solutions & UNamur

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Current situation

INNOVATIVE COATING SOLUTIONS
www.incosol4u.com

- 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

https://www.incosol4u.com/modeling-and-simulation

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

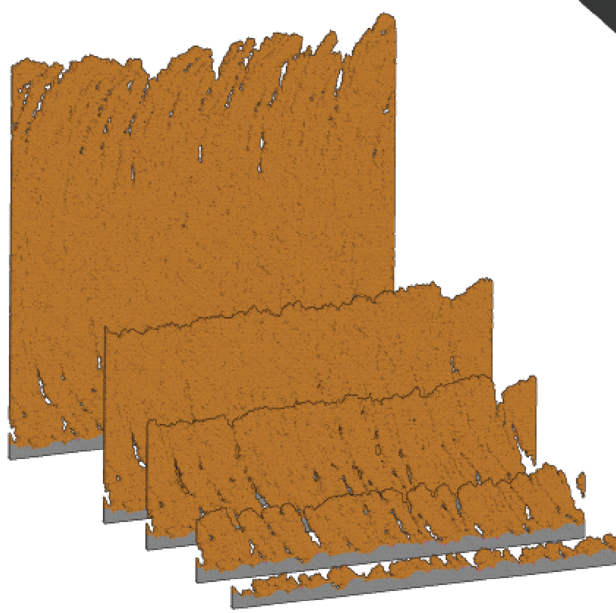
INNOVATIVE COATING SOLUTIONS

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.

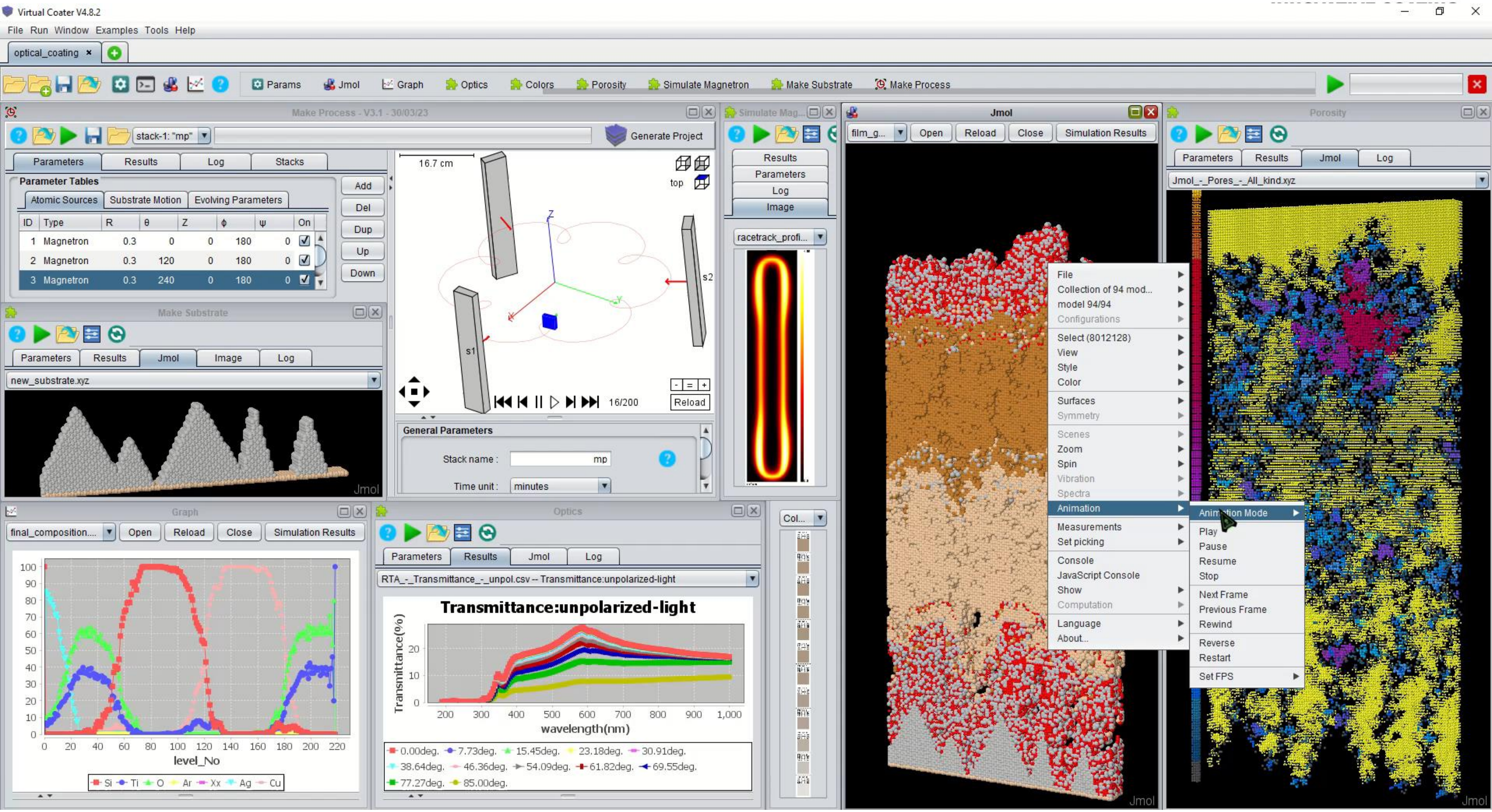


3. ANALYZE

Virtual Coater™ analyses the propreties 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.)



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Virtual Coater

- « 2D substrates »: validated

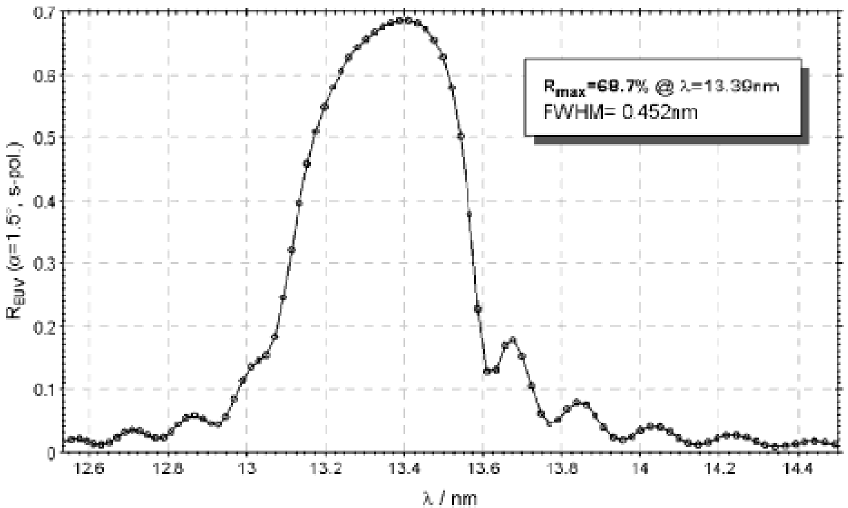


Figure 44: EUV reflectivity of pure Mo/Si-multilayers (dperiod = 6.82 nm, = dMo/dperiod = 0.39, number of periods N = 65) prepared by MSD (Figure 1 in ref. 4).

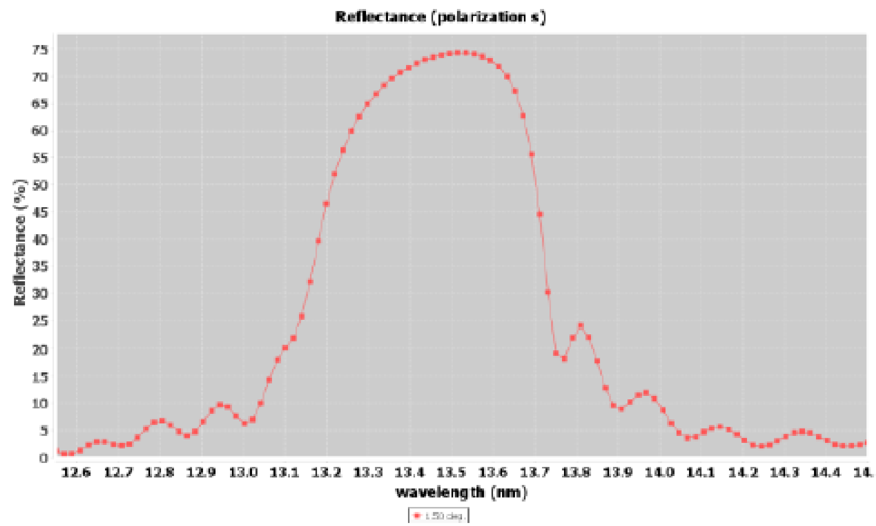
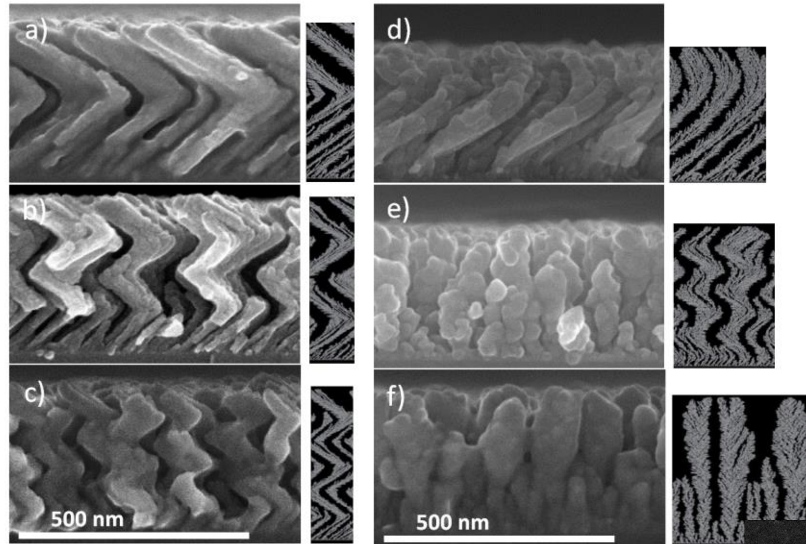
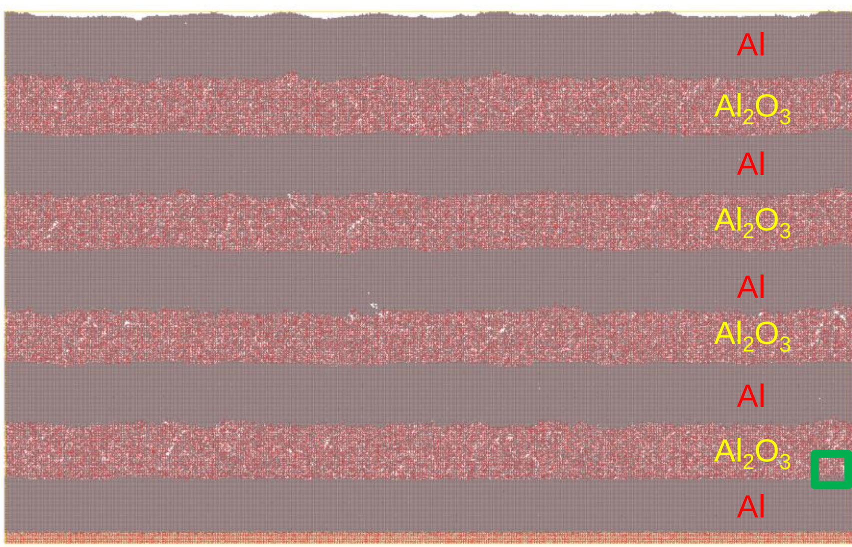


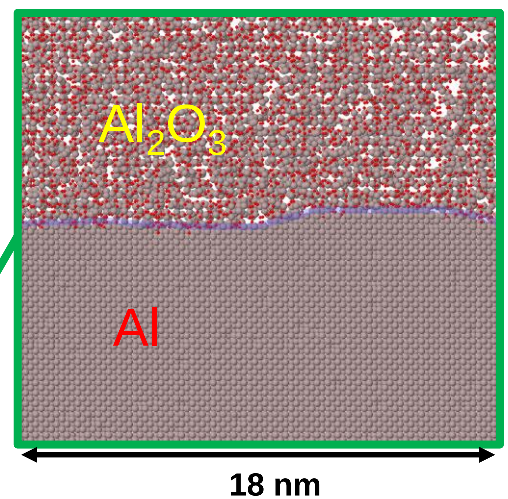
Figure 45: EUV reflectivity of simulated deposition of Mo/Si-multilayers and computed by the *Optics* plugin.

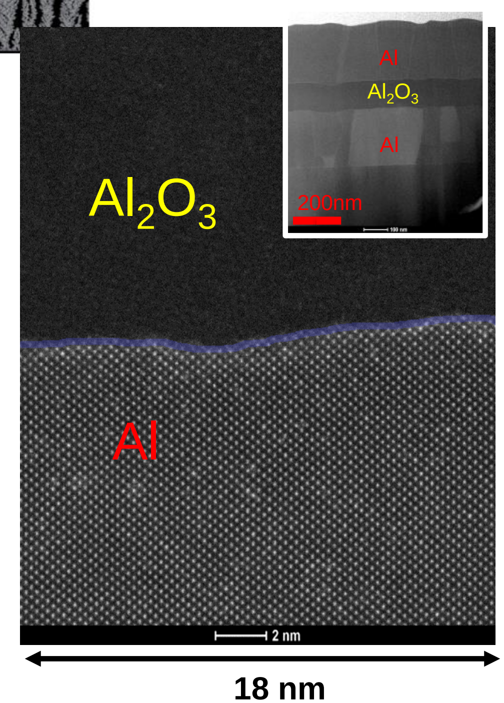
Virtual Coater

- « 2D substrates »









iCS INNOVATIVE COATING SOLUTIONS
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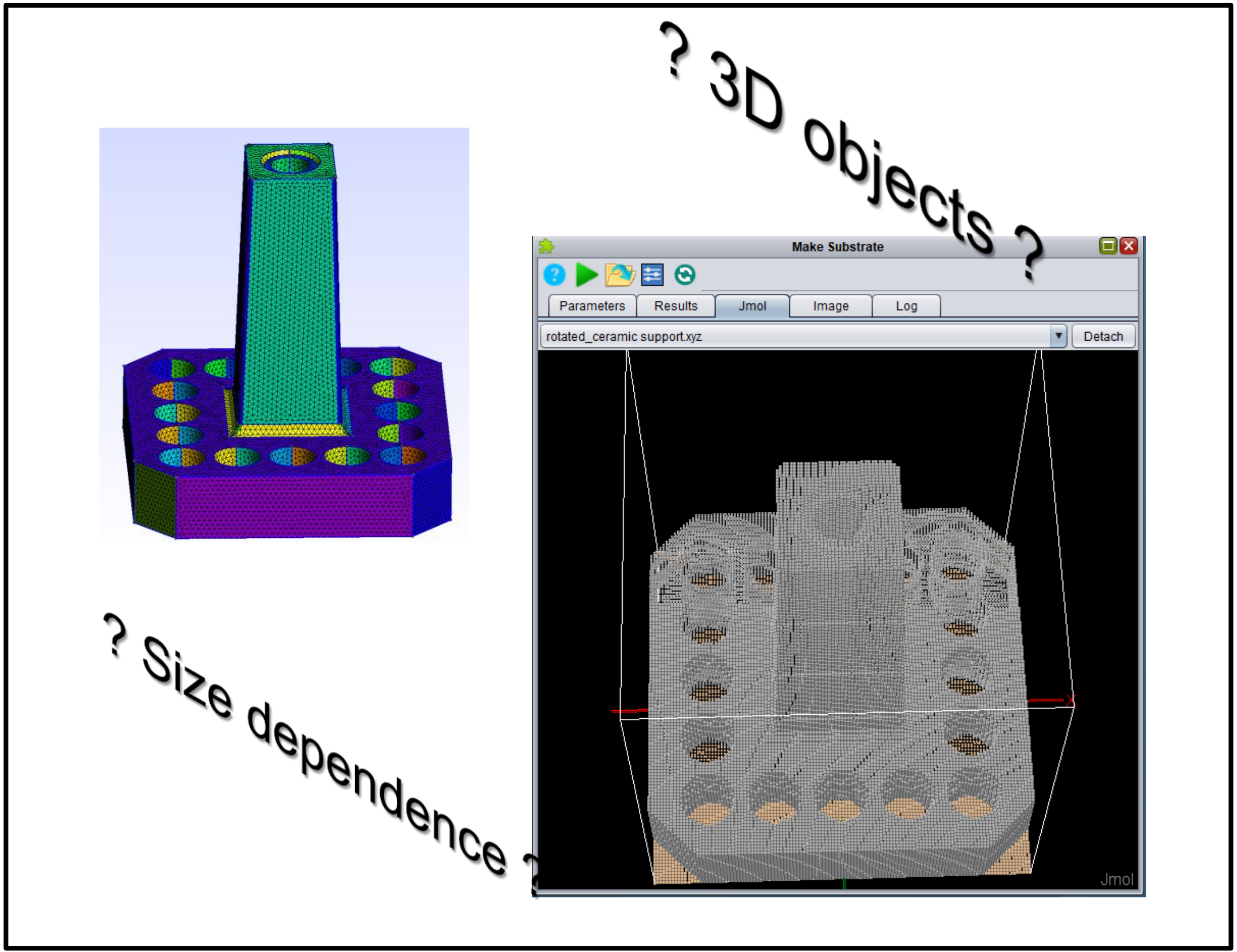
Virtual Coater

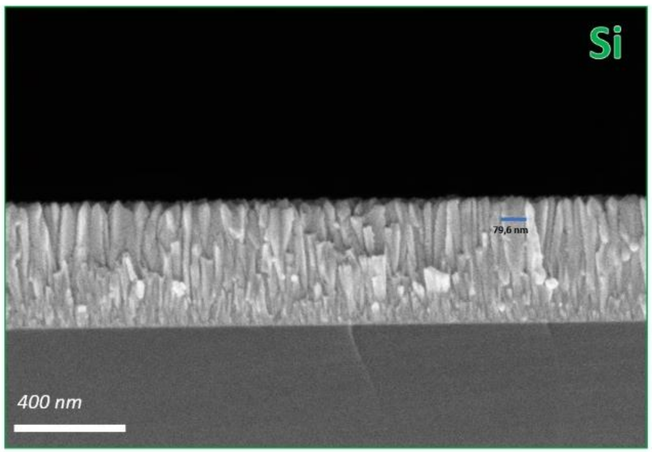
- What about 3D substrates ?

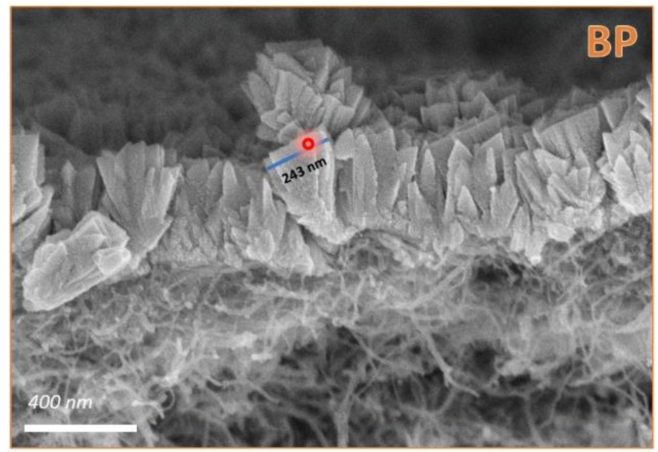


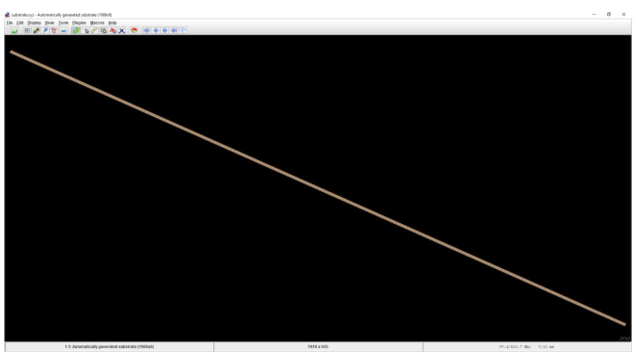
Reactive magnetron sputtering dep. on buckypaper

<u>Studied Substrates</u>:

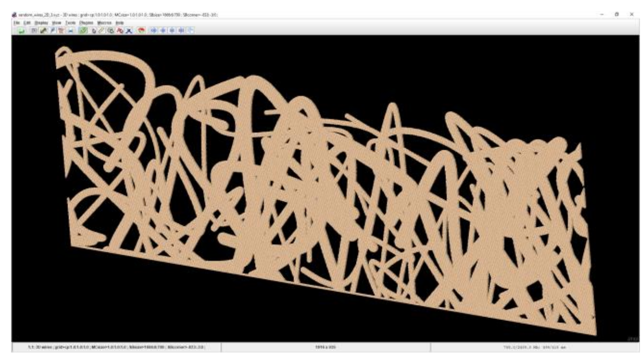
- Comparison flat substrate VS buckypaper
- 3D simulations (500nm x 3nm x 400nm)
- Scale: 1:1 (1 atom = 0.2 nm)







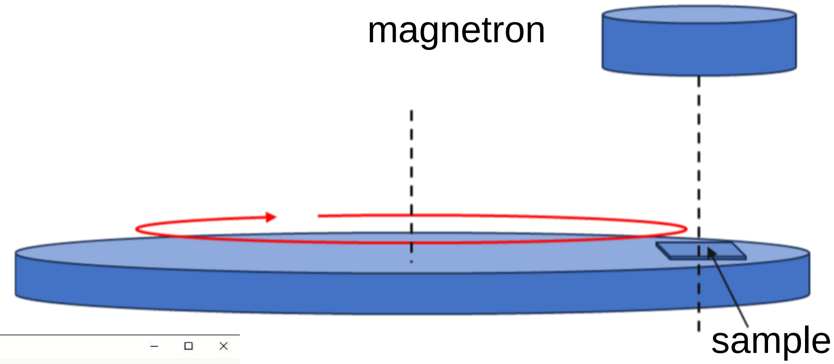
Si flat substrate

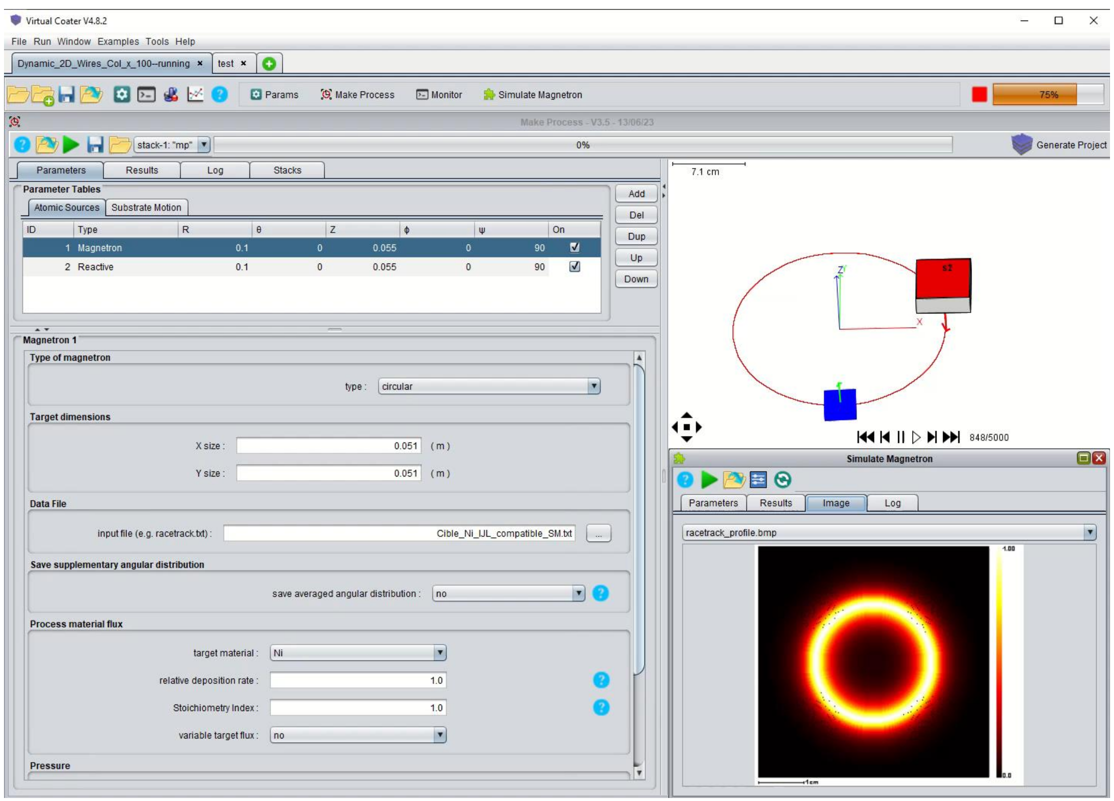


C Buckypaper substrate

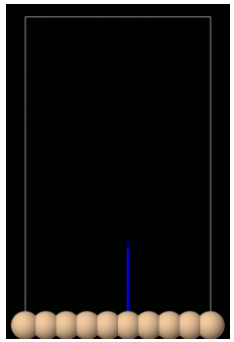
Reactive magnetron sputtering dep. on buckypaper

<u>Deposition process</u>:
- MeN deposition by RSD
- rotation of the sample (>3000 loops)



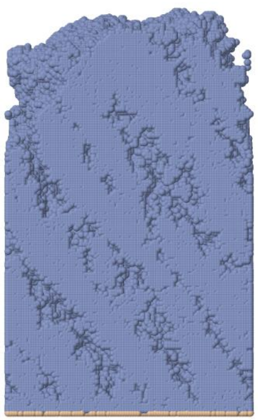


How to visualize Columns ?

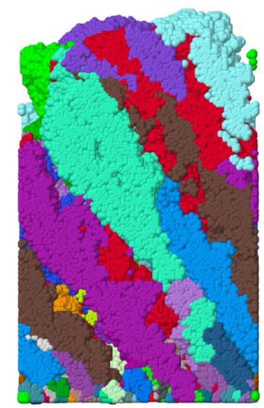


History (deposition relocating)

Column identification

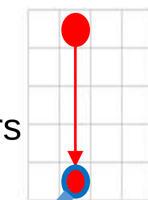


Based on the nearest neighbors (deterministic method)

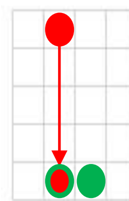


Virtual Coater simulation of a Me film

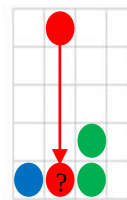
No neighbours

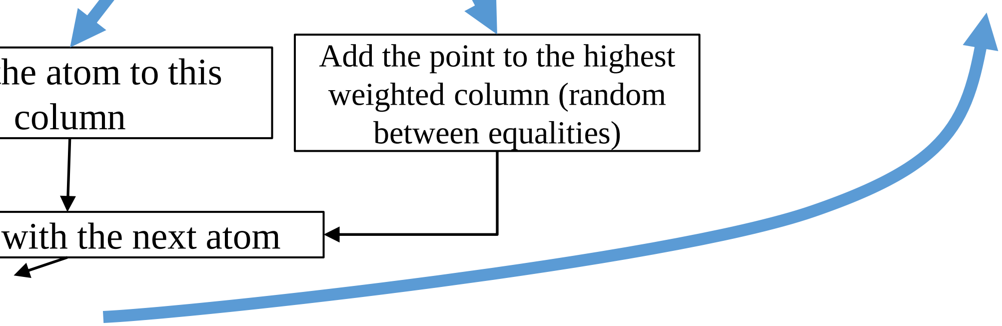


Neighbors from the same column



Neighbors from different columns





Create a new column

Add the atom to this column

Add the point to the highest weighted column (random between equalities)

Continue with the next atom

…

Aurélien Besnard / Noé Watiez

Reactive magnetron sputtering dep. on bucky

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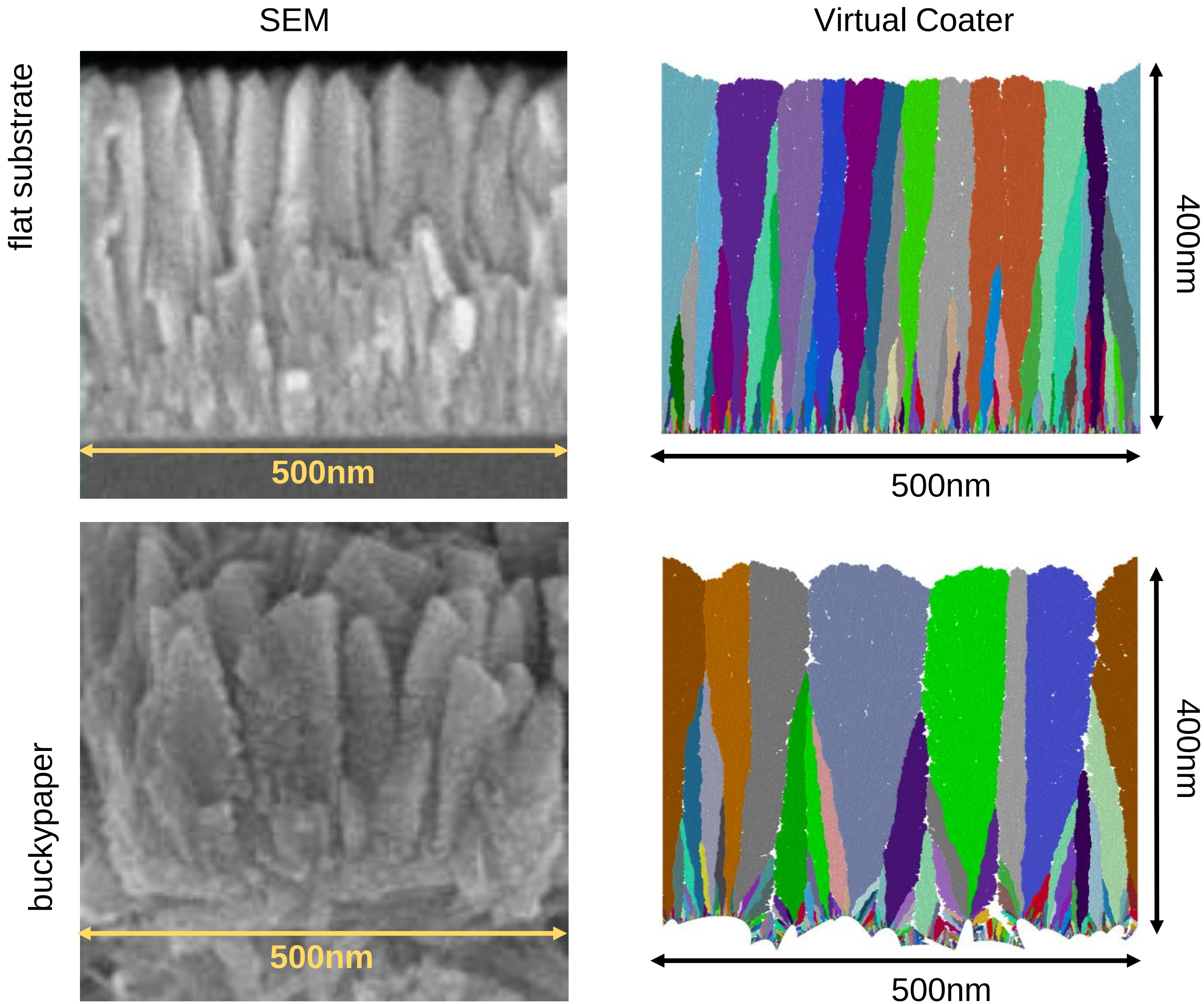
Film growth and column detection:

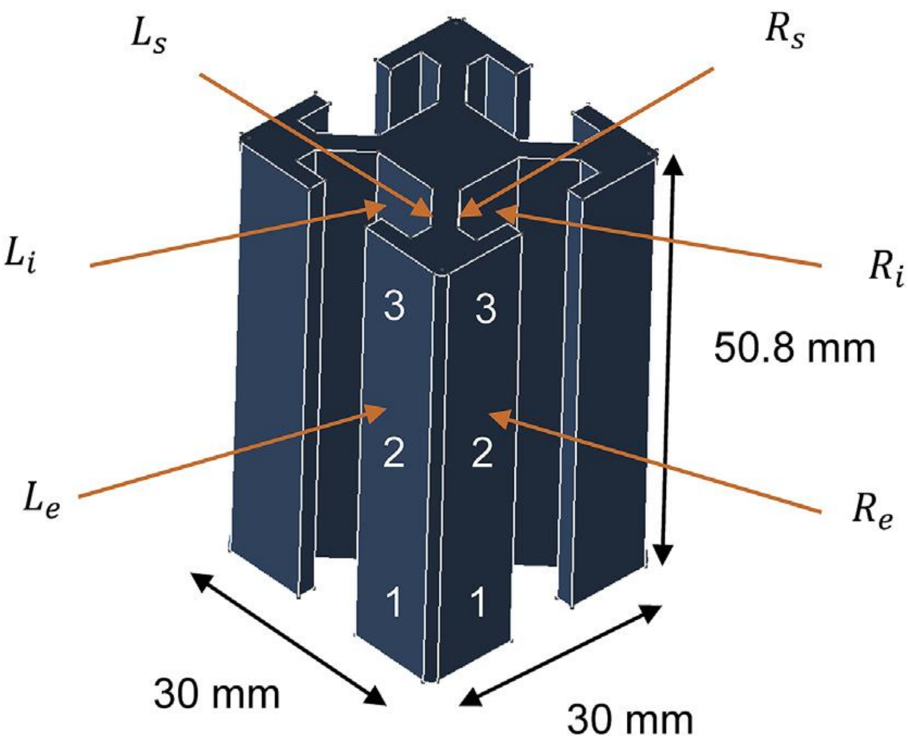


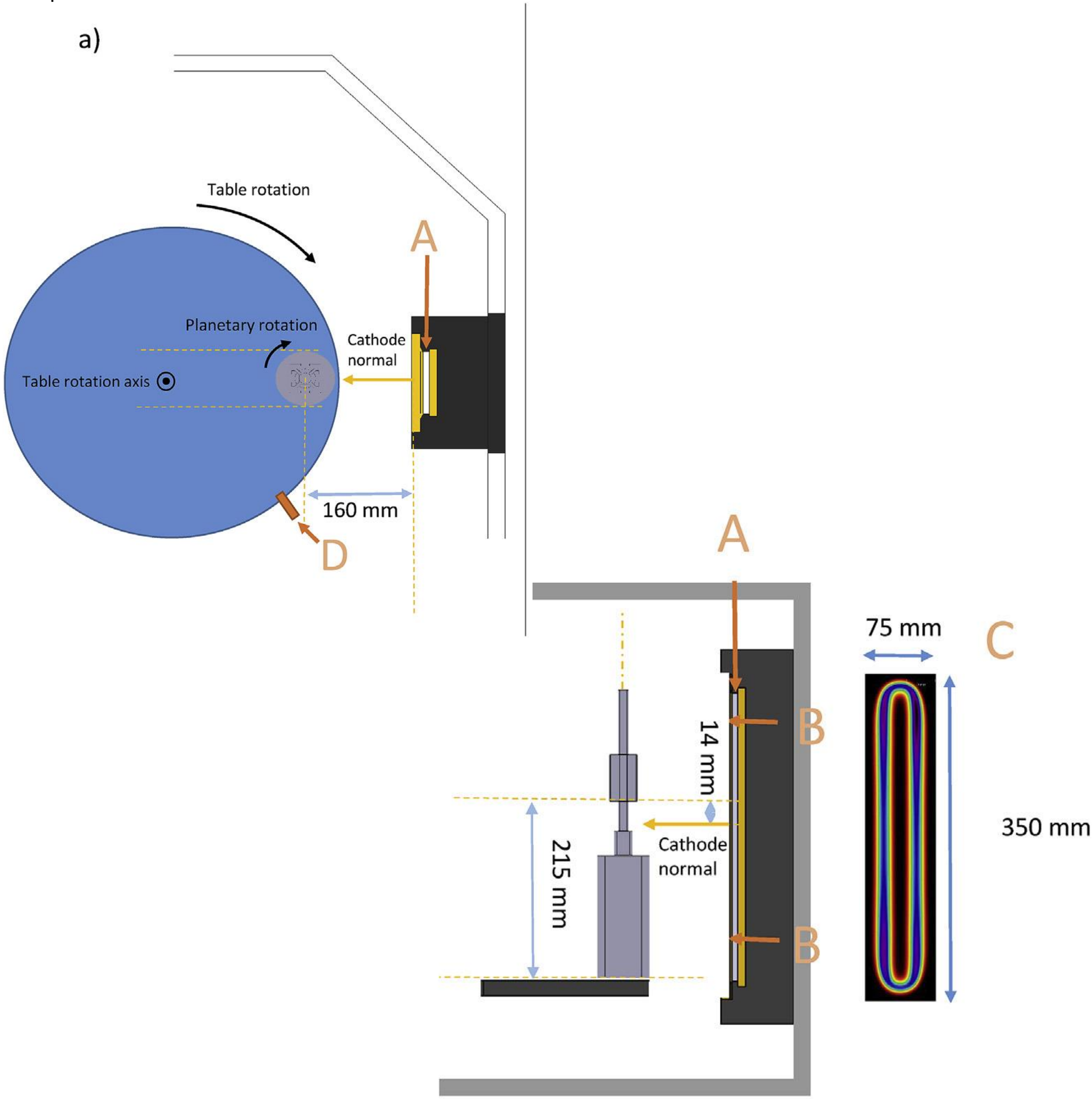
Study of the influence of the pressure and rotational motion of 3D substrates processed by magnetron sputtering: A comparative study between Monte Carlo modelling and experiments

Martin Evrard[a], Aurelien Besnard[b], Stephane Lucas[a,*]

[a] University of Namur, LARN-NISM, 61 rue de Bruxelles, B-5000, Namur, Belgium
[b] Arts et Metiers ParisTech, LaBoMaP, Rue porte de Paris, F-71250, Cluny, France

Surface & Coatings Technology 378 (2019) 125070





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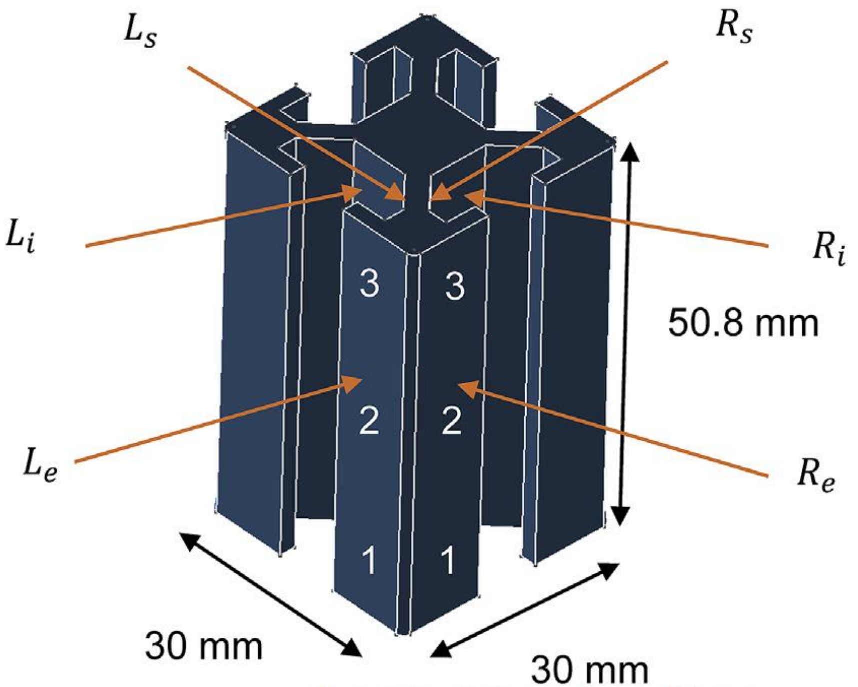
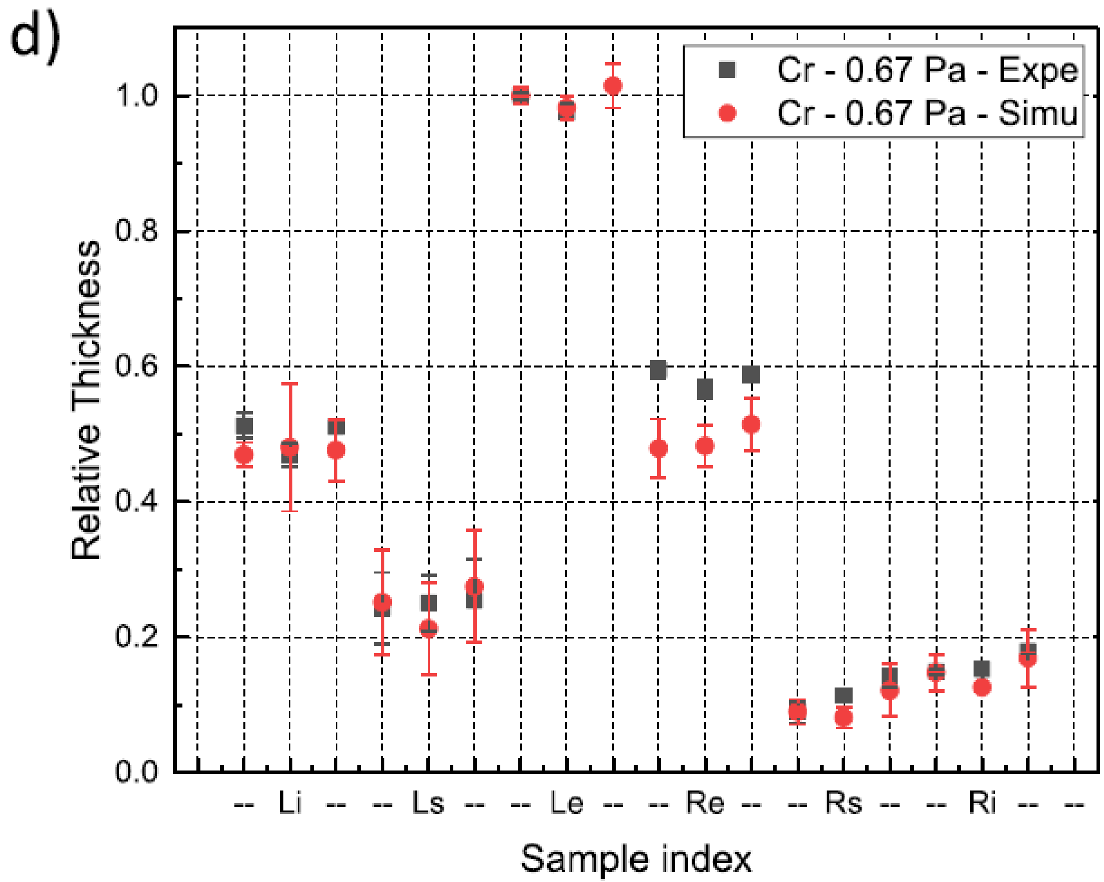


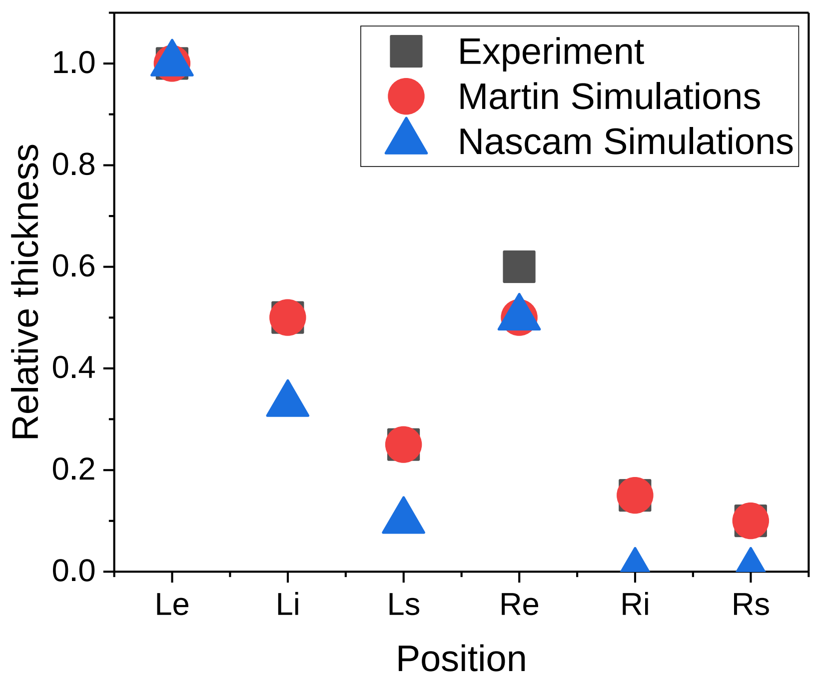
Fig. 4. Meshing of substrate and space cellularisation.

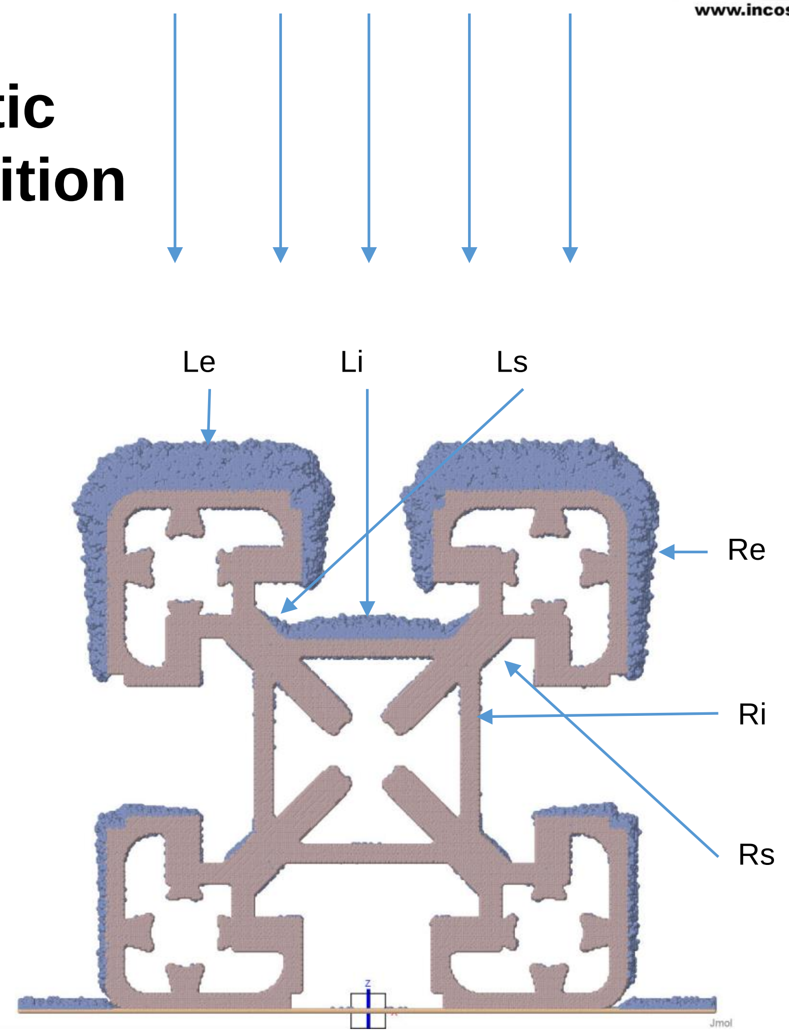


Deposition on 3D mm sized parts

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
<u>300x300x400: 1 atom = 100 µm</u>

Static deposition

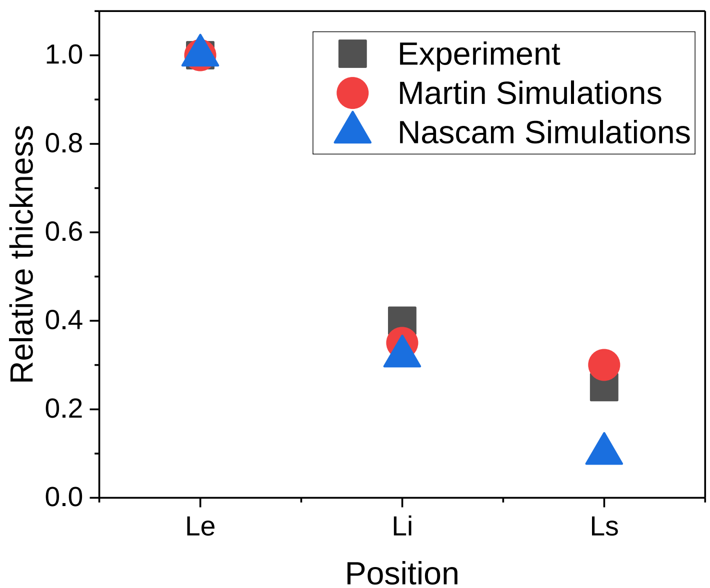




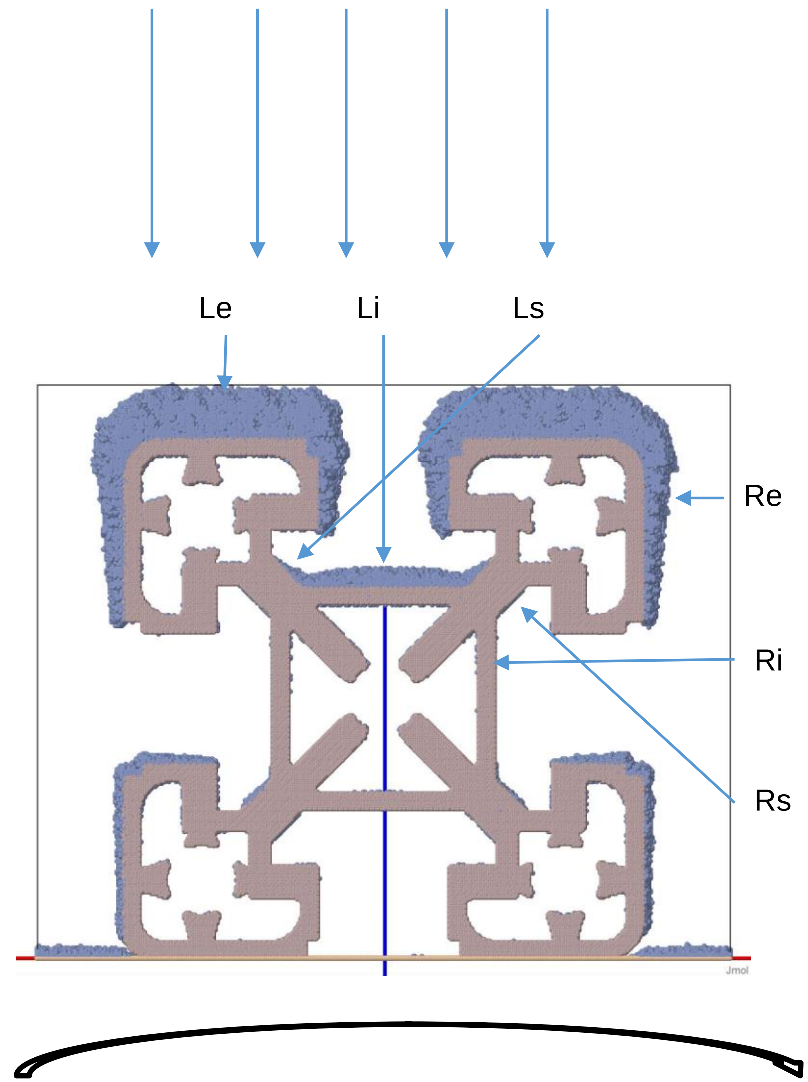
Deposition on 3D mm sized parts

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

<u>300x300x400: 1 atom = 100 µm</u>

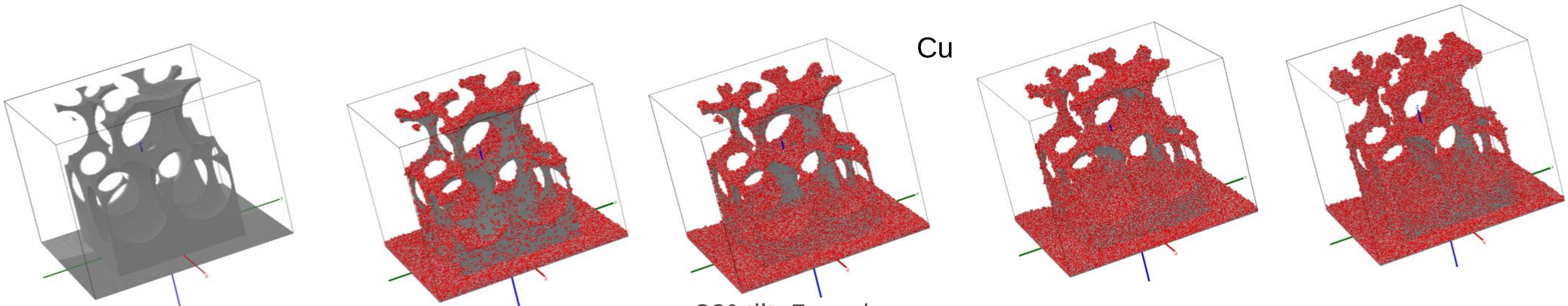


1-fold rotation deposition



Other cases

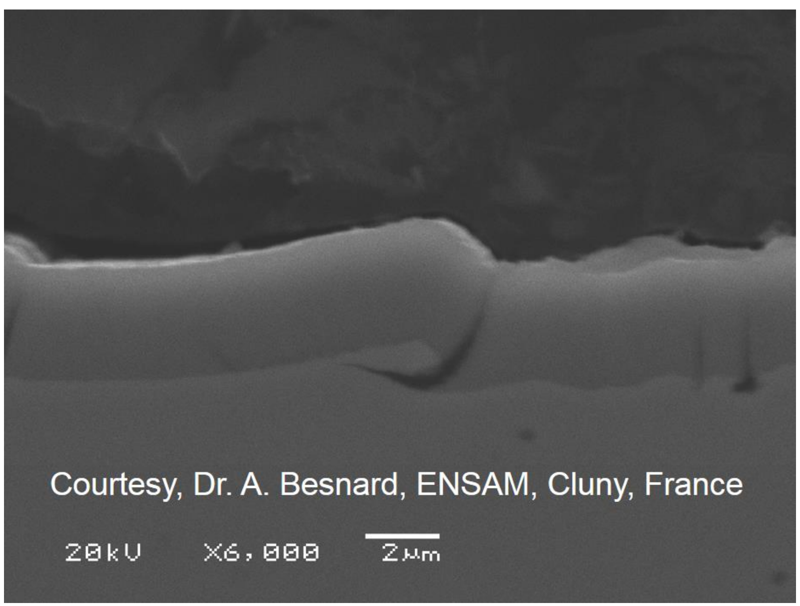
Real foam : 2.5mm ; 1 atom ≈ 10 µm



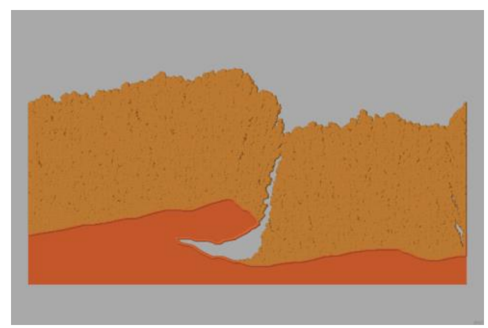
30° tilt, 5 osc/s

60° tilt, 5 osc/s

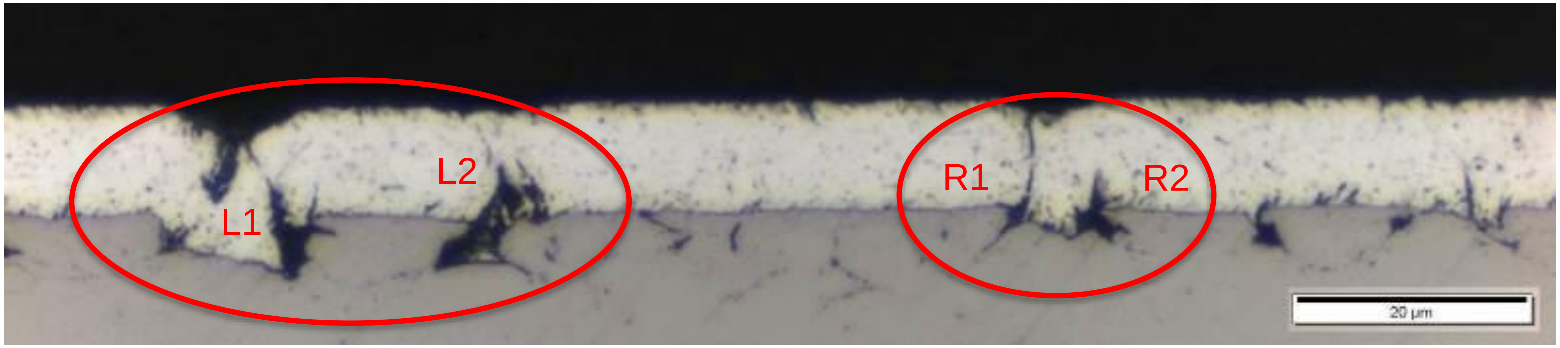
90° tilt, 5 osc/s

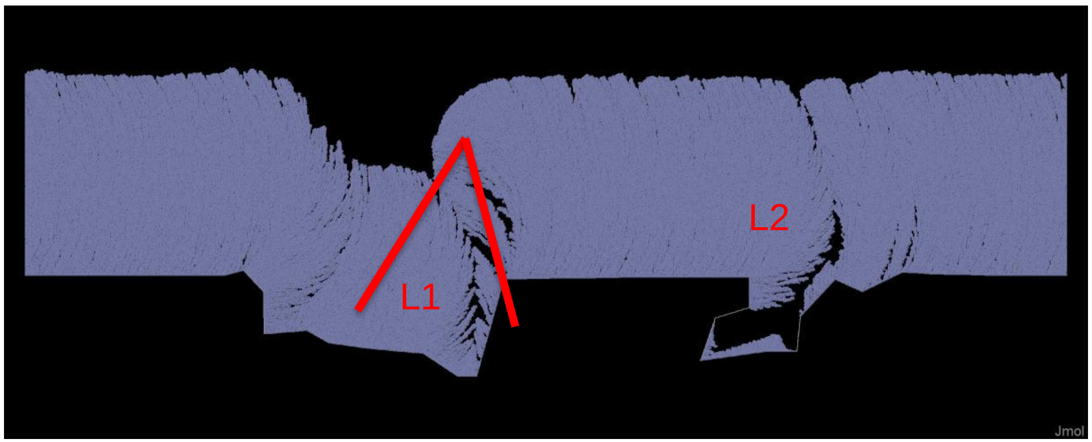


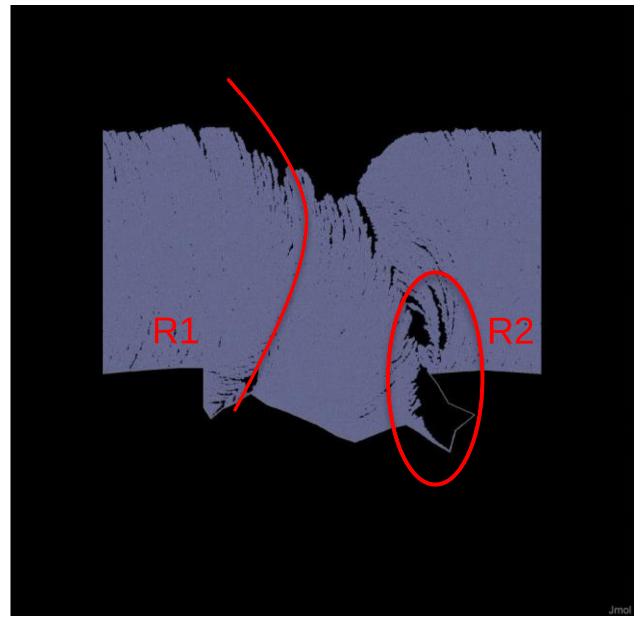
465 atoms : 12 µm / 1 atom ≈ 40 µm



Other cases



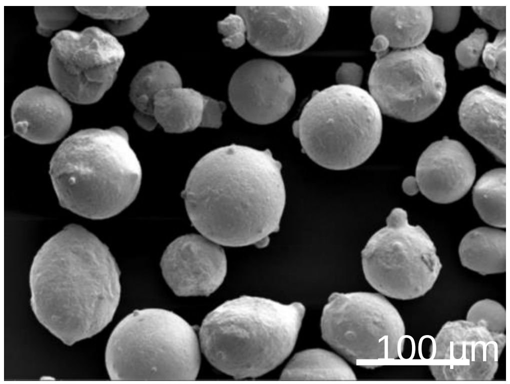




We helped the customer to understand the following:

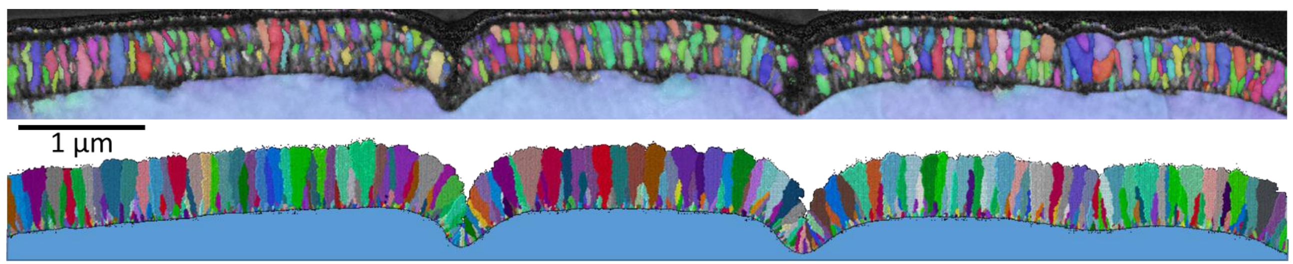
- What is the effect of the moving strip speed and the deposition rate ?
- What is the effect of pressure ?
- What is the effect of strip temperature ?
- What is the effect of source divergence ?

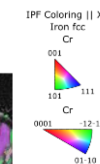
Other case



Cr deposited on 316L particles

TKD analysis on a FIB slice





1 at = 4 nm

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

Courtesy Prof. A. Besnard, ENSAM, Fr

Summary

INNOVATIVE COATING SOLUTIONS
www.incosol4u.com

- 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. !***

Case	***1 atom ≈***
Bucky paper	$2x10^{-4}$ µm
Zn defects on Steel	1 µm
Foam	10 µm
Cu defects on Steel	40 µm
Metallic profile	100 µm

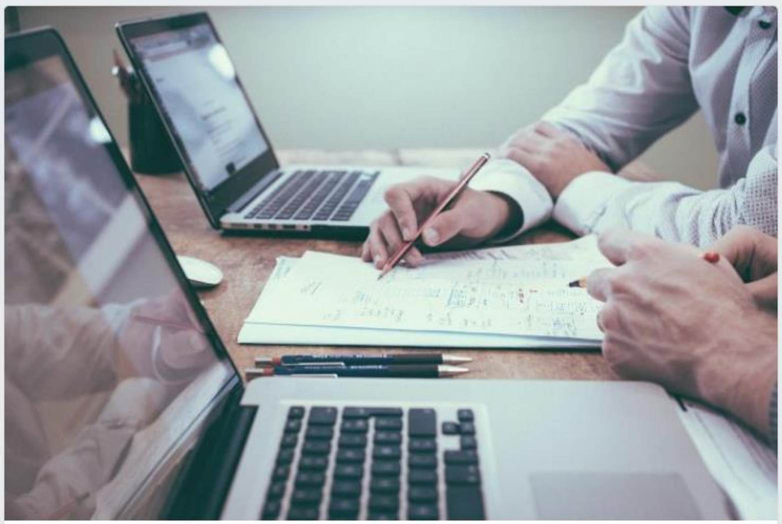
- ***The only main limitation know today is hidden surface facing the incident direction***

Many Thanks

slu@incosol4u.com / www.incosol4u.com

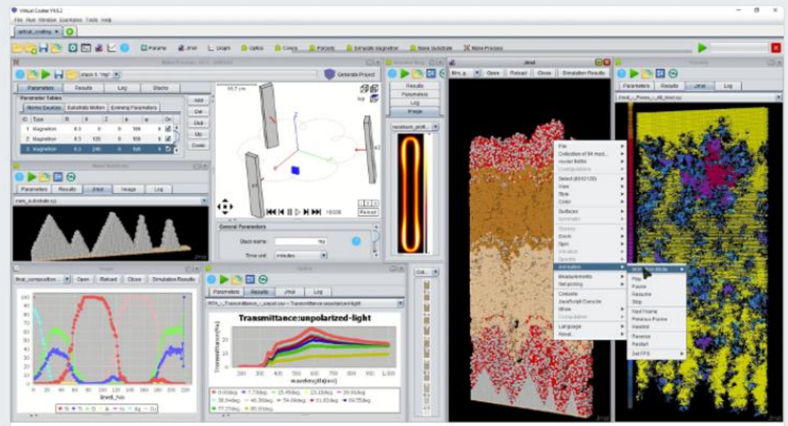
Modeling and simulation

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