Finite element mesh generation for nano-scale modeling of tilted columnar thin films for numerical simulation

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Introduction

The PVD, process produces coatings with columnar morphology. In GLAD technologies, the columnar aspect is even more pronounced and becomes a major factor in the properties of the film.

In this study, a GLAD simulation is run and additional tools are developed to better take into account the columnar morphology of the film:

- Columns identification algorithm → Compute a column segregation from a simulated coating.
- Construction of mesh for each column → Opens the way for a column comprehensive finite element analysis of the film.
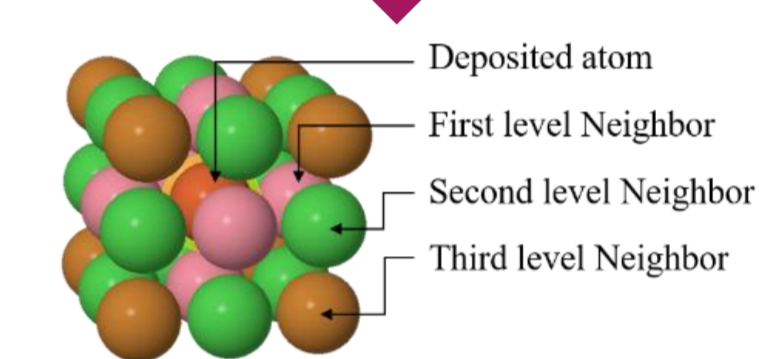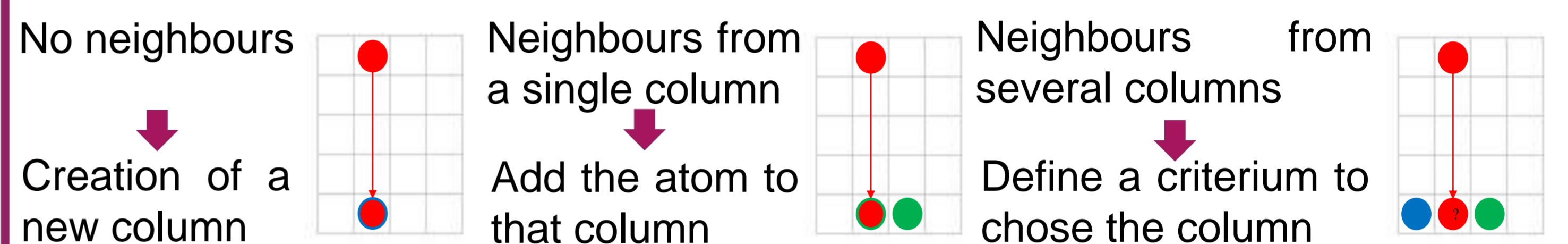
Initial simulation steps

The simulation is run for Cr films at different incidence angles.

- SRIM is used to compute the sputtering depending on the substrate composition and the ion flux.
- Then SIMTRA is used to simulate the transportation of the particles in the chamber. The sputtered particle flux is determined by using SRIM data along the racetrack extracted from a used target.
- Finally NASCAM is used to compute the growth of the film on the substrate based on transportation data.
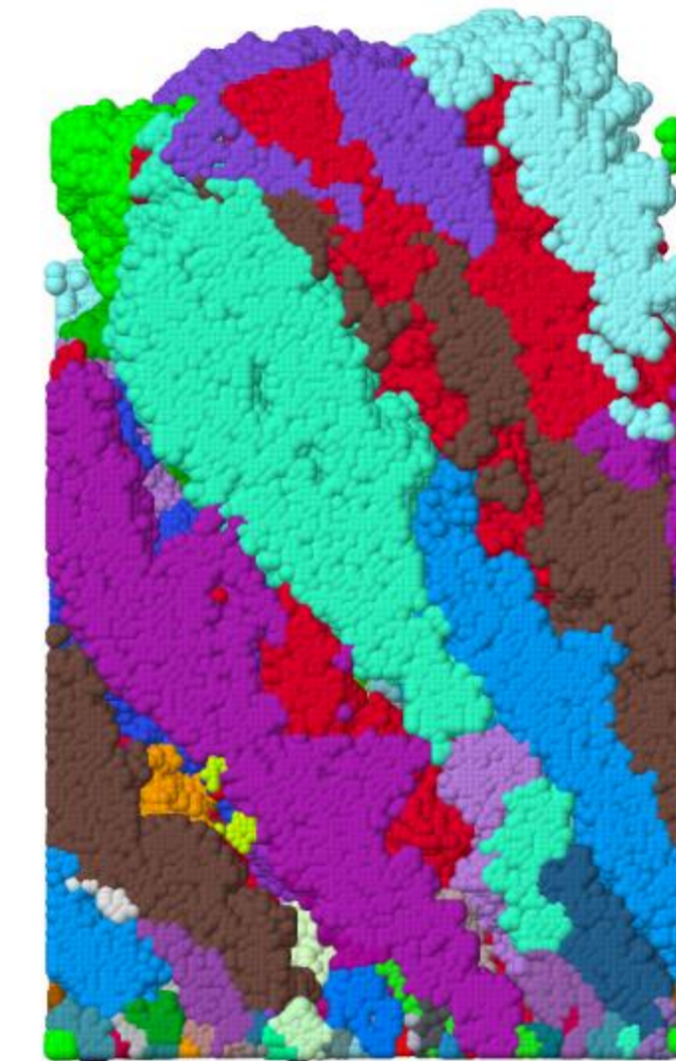
Example of a Cr coating simulated for an incident angle of 50°

Mesh construction

Unravelling the periodicity of the coating simulated by NASCAM
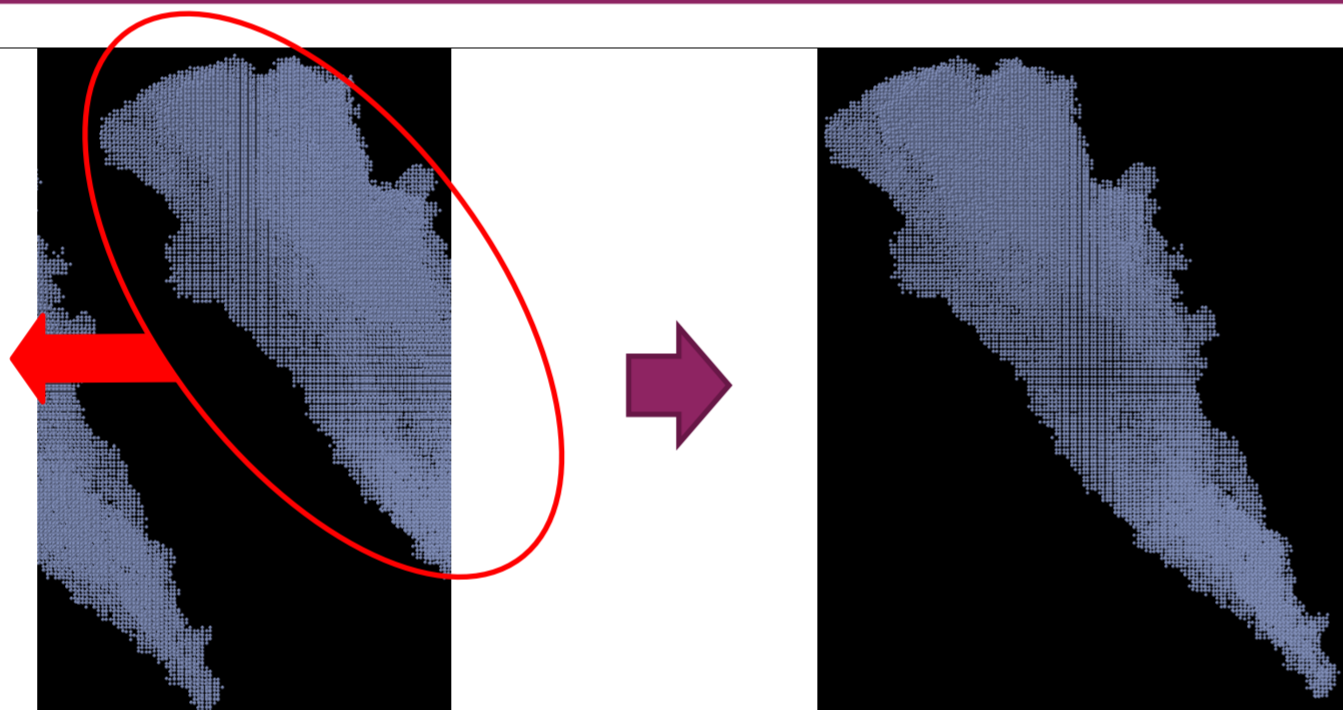
Steps for the mesh construction (visualisation by 2D slices)

Selection of the column

Export of the pointcloud

Filling the holes in the columns

Creation of the mesh

Correction and smoothing of the mesh

3D visualisation of the mesh

Assembly of all the columns mesh for the Cr coating

— 100 nm
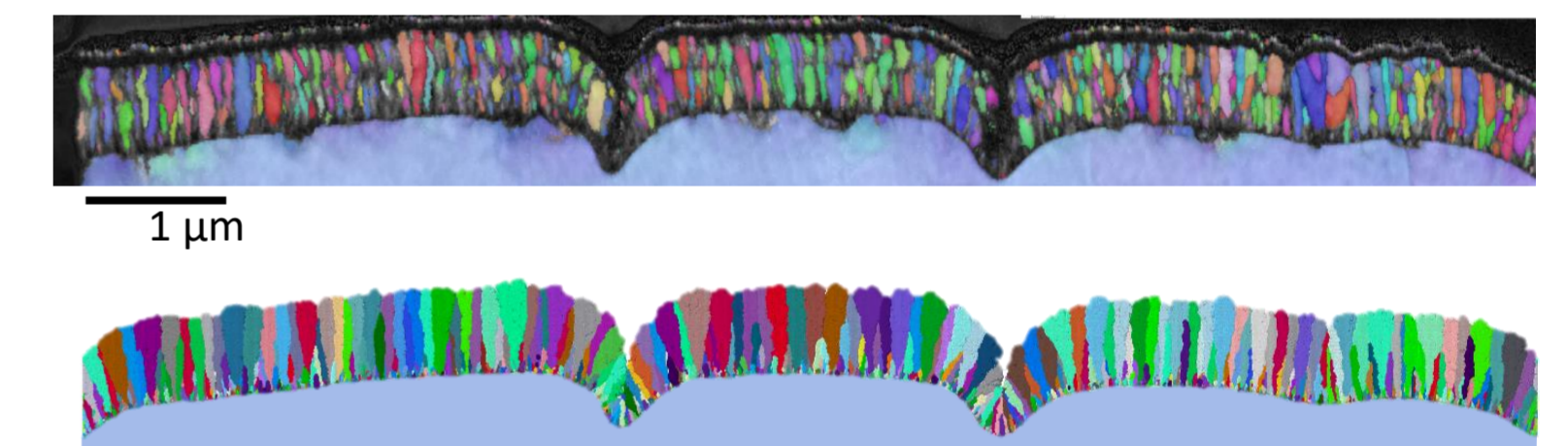
Column identification algorithm

This algorithm is derived from the historicity of the deposition in the simulation. For each deposited atom, its neighborhood is checked at the time of deposition. Three situations were identified:

No neighbours
Creation of a new column

Neighbours from a single column
Add the atom to that column

Neighbours from several columns
Define a criterium to chose the column

Deposited atom
First level Neighbor
Second level Neighbor
Third level Neighbor

Weight added to each column depending on the number of neighbouring atoms and their distance

Cr coating simulated for an incident angle of 50° with column identification
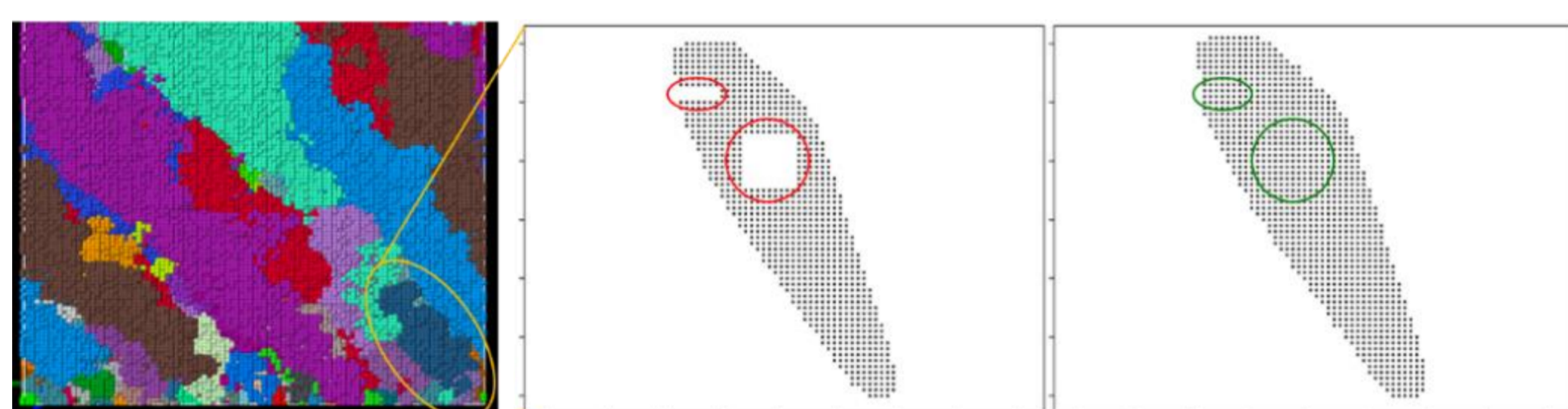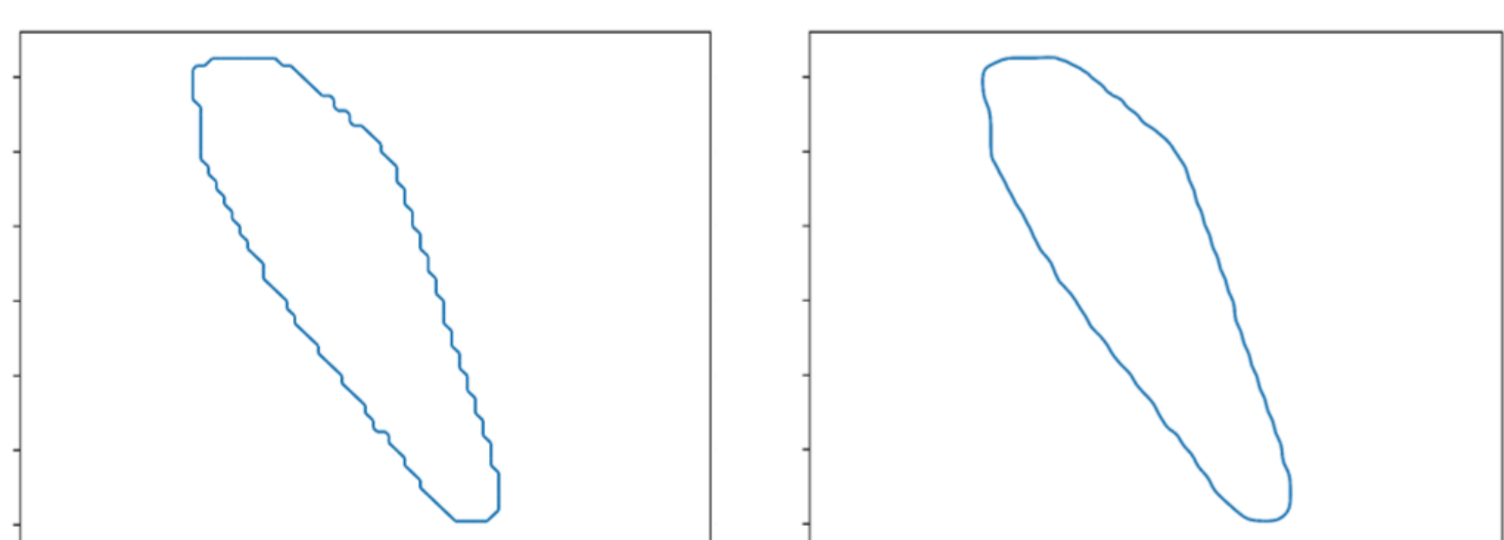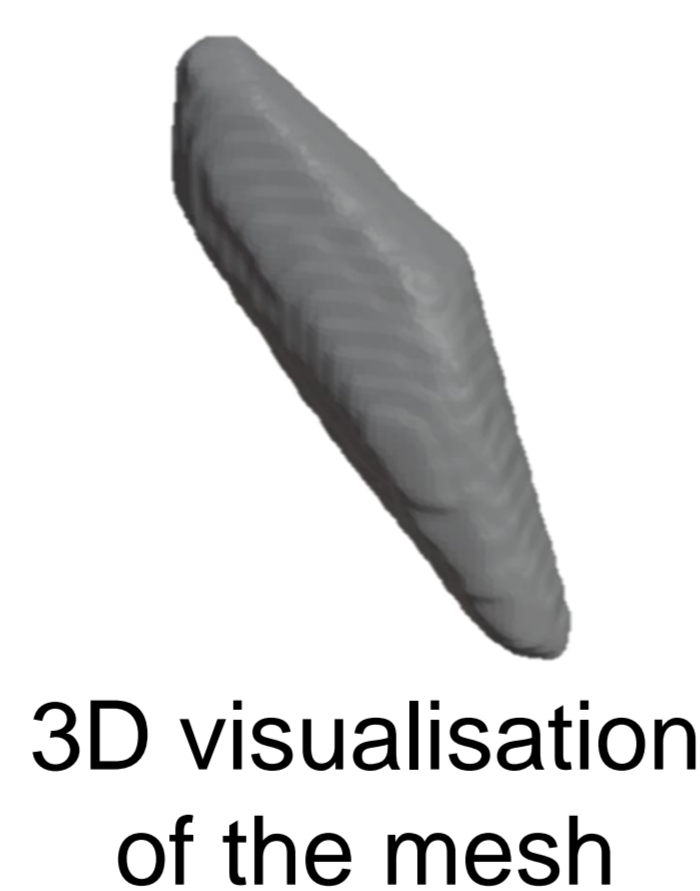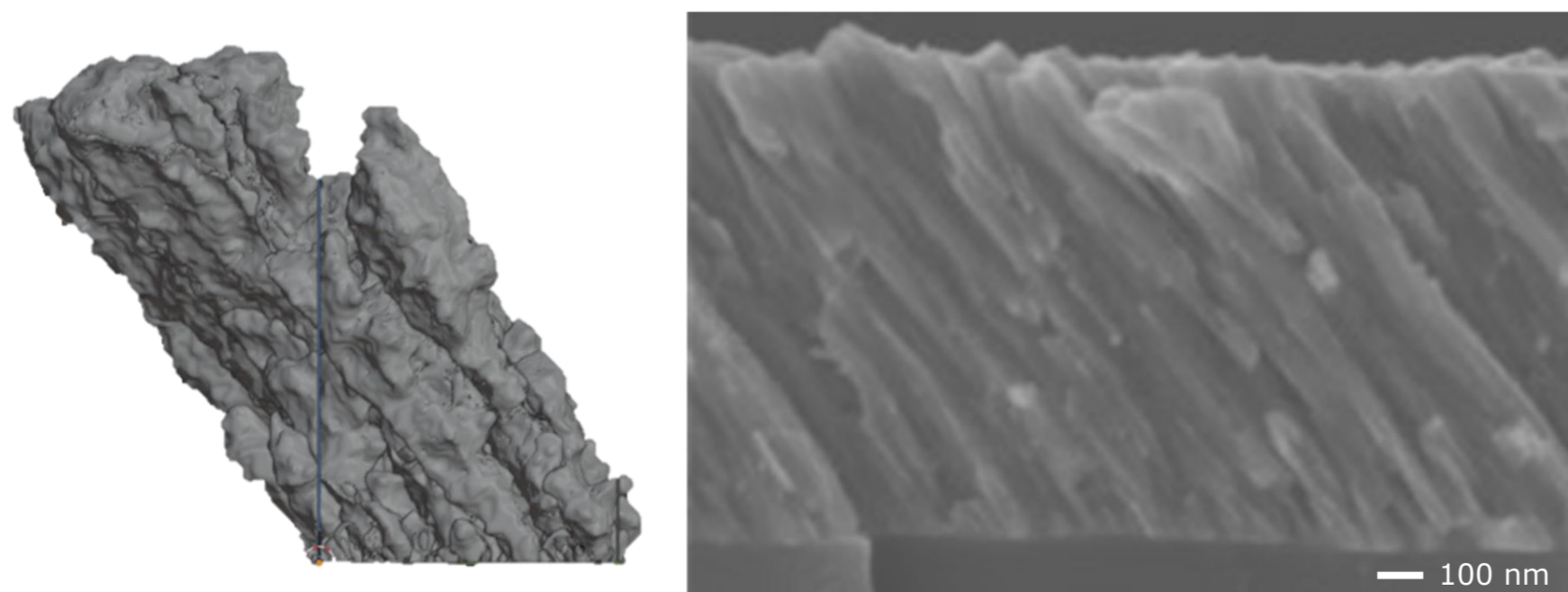
1 µm

Comparison between an EBSD image and a simulated film with column identification for chromium deposition

Using the column identification for analysis :

- Slicing the film around the columns
  Show the columns roughness on the slice, closer to a physical slice than a perfect cut along the grid axis.

- Analysing a single column at a time
  Produces data on the size, shape and angle of each individual column

- Exporting statistics of the film based on the atoms or the columns
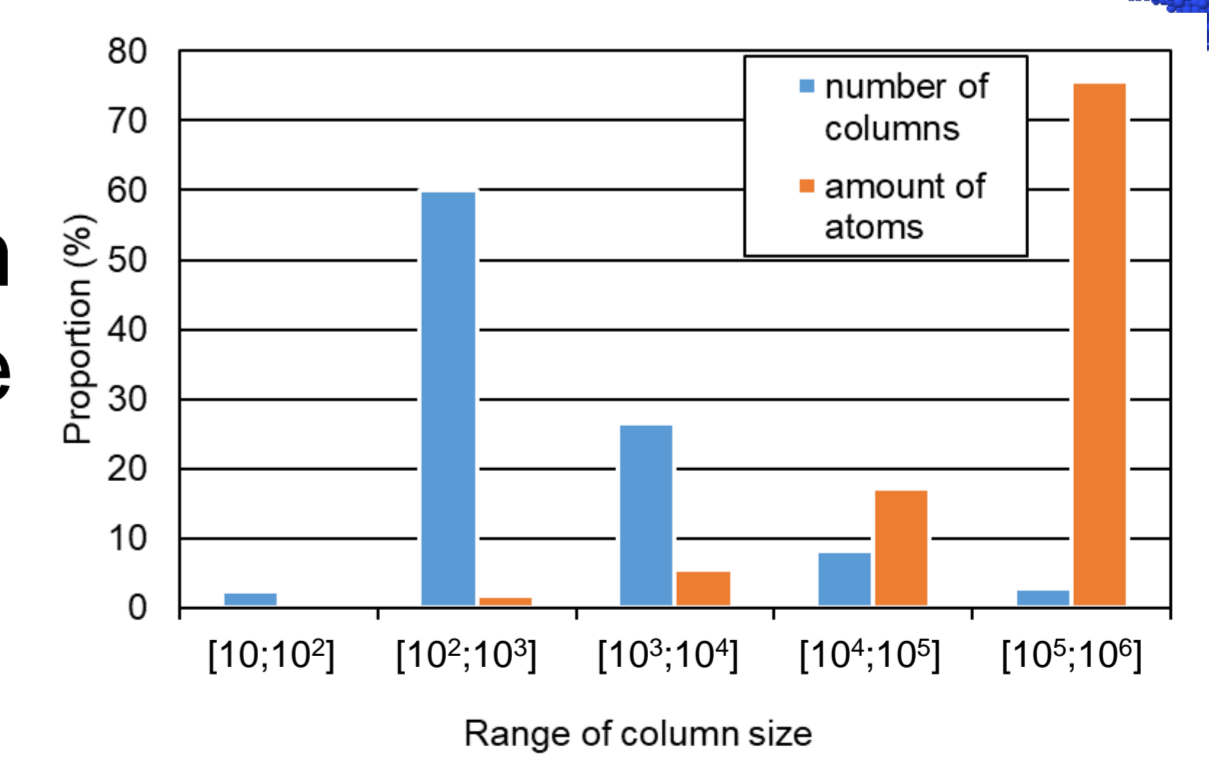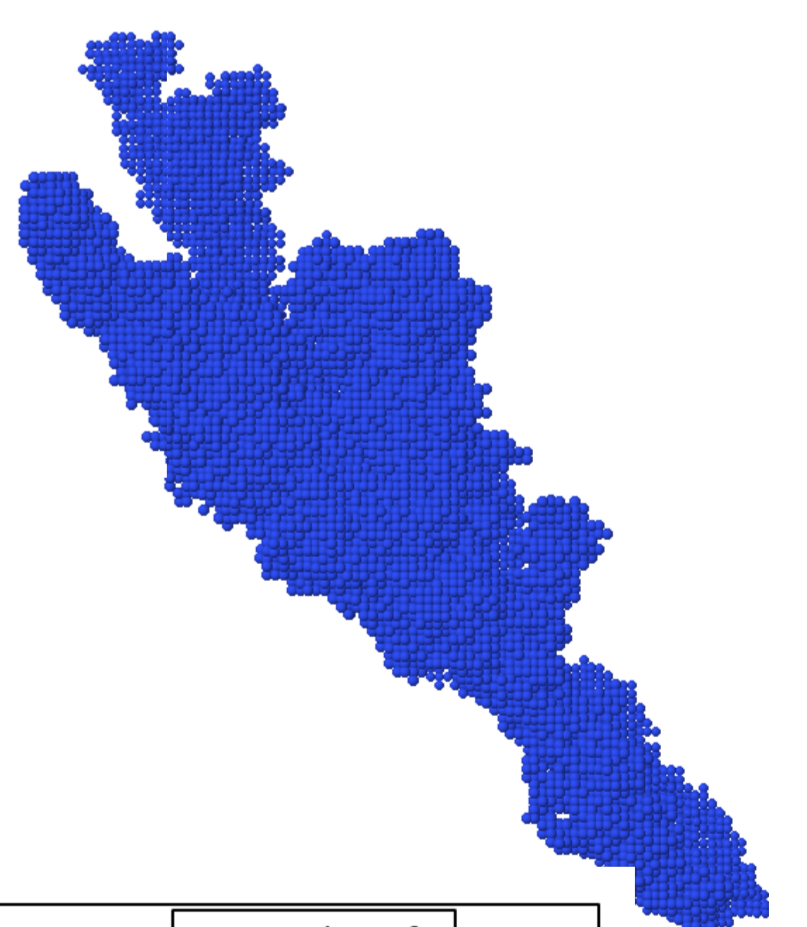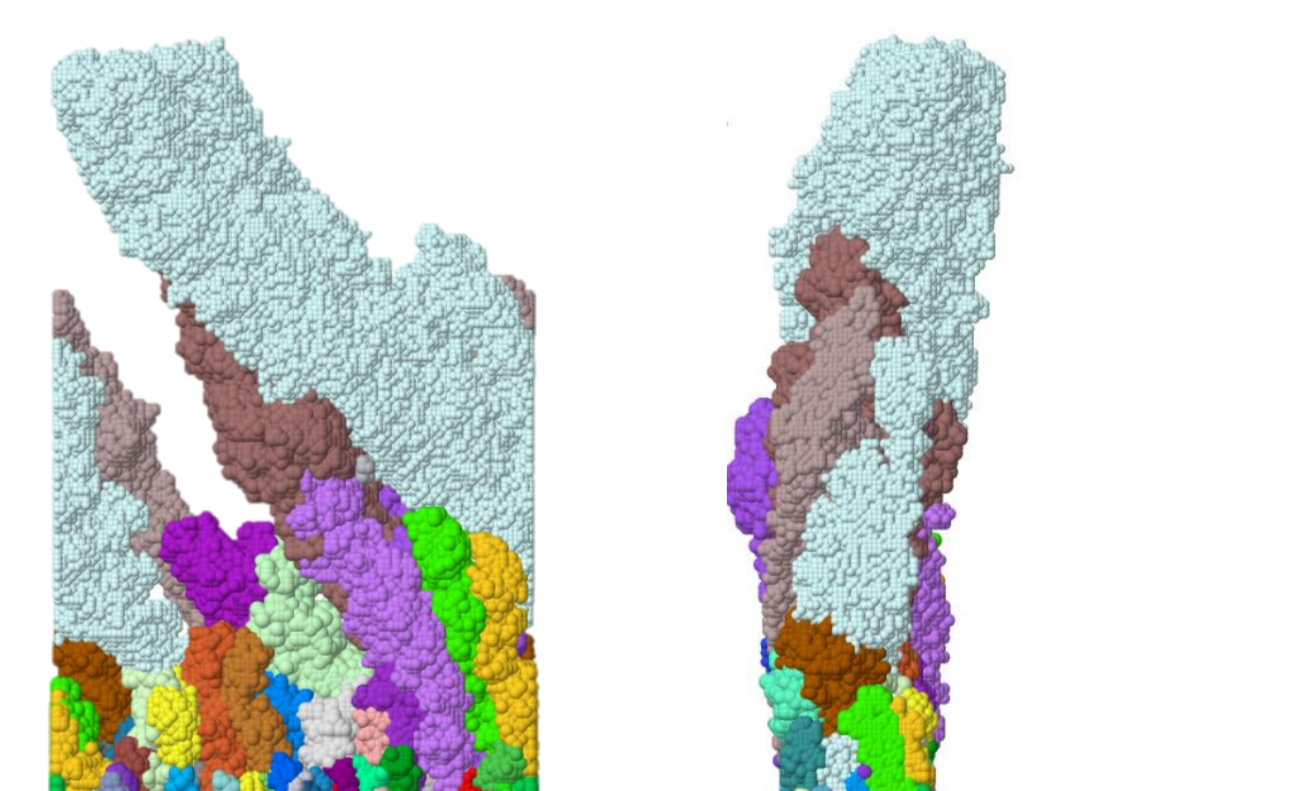
Conclusions

- The comparison between the EBSD and the simulated film tends to validate the Column identification algorithm.
- This algorithm is not only a necessary step towards the mesh construction but also enable more precise and repeatable analysis of the simulated films.
- The constructed mesh show a good accordance in both column shape and angle compared to the SEM image.
- The column meshes are ready for FEA computation. It is now necessary to evaluate the interaction between each column for the full mechanical computation