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Analyse of the angular distribution of the columns of chromium tilted thin films through a comprehensive simulation

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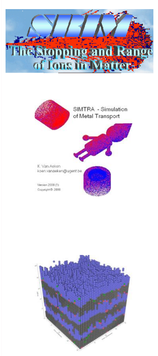
Introduction

PVD coatings present a columnar morphology. With the OAD process, this columnar aspect is even more pronounced and has a significant influence on the properties of the film. Consequently, an accurate and robust evaluation of the column tilt angle is needed. Nowadays, the measurement is performed from 2D cross-section images (SEM or simulated). This study aims to develop a statistical evaluation of the angle of a simulated coating taking into account all the columns. For this purpose :

- Firstly, a methodology is defined for the measurement of the angle of the individual columns.
- Secondly, the measurements are analysed statistically in order to deduce the angle of the coating.

Simulation steps

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



- SRIM computes the **sputtering process** depending on the substrate composition and the ion flux.
- SIMTRA simulates the **transportation** of the particles in the chamber, based on the SRIM data and the racetrack profile.
- NASCAM compute the **growth of the film** on the substrate based on transportation data.
- Finally, a home made algorithm*, provides the **columnar morphology** of the film as either a list of point clouds or a list of meshes.

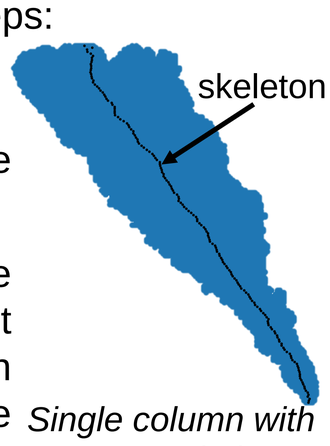
* Watiez, N. *et al.* (2023). Finite Element Mesh Generation for Nano-scale Modeling of Tilted Columnar Thin Films for Numerical Simulation, PLM 2022

Measurement of the angle of a column

As a coating is composed of thousands of columns of different sizes, a reliable methodology for the measurement of the angle of each column, has to be defined. It should also be applied, either to a point cloud or to a mesh.

The methodology has been devised in three steps:

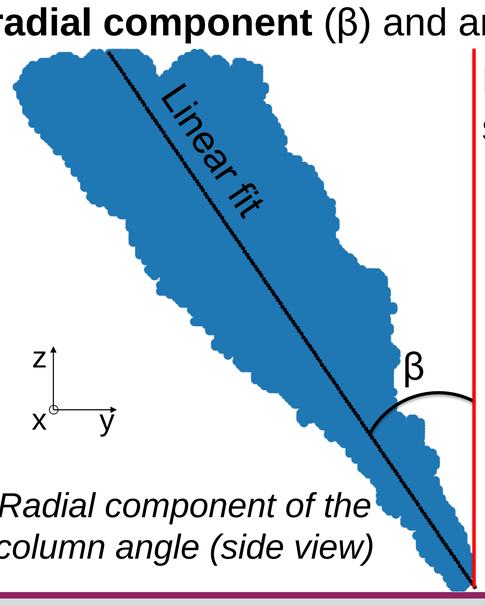
- extract a **skeleton** from the structure.
- approximate the skeleton with a **line**
- measure the **angle** between the line and the normal of the substrate.



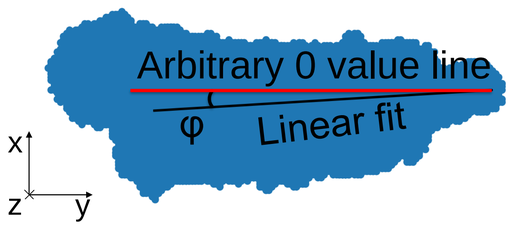
Single column with apparent skeleton

The **skeleton** is defined here as a curve passing through the **middle of the column**. It is constructed by slicing the column horizontally and calculating the centroid of the points contained in each slice.

A **linear fit** is then applied to the skeleton to represent the principal direction of the column. The **angle** is separated between a **radial component** (β) and an **azimuthal component** (φ).

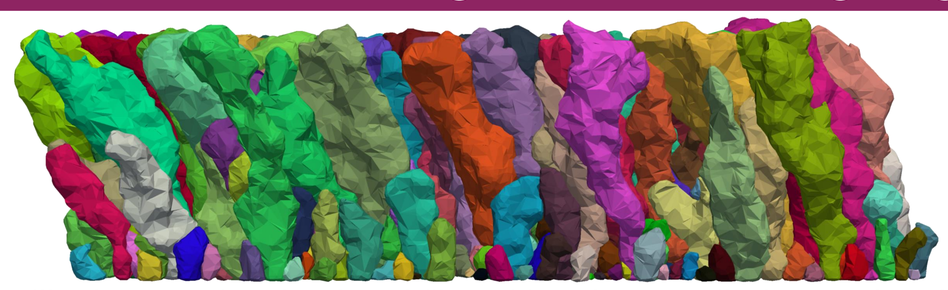


Radial component of the column angle (side view)



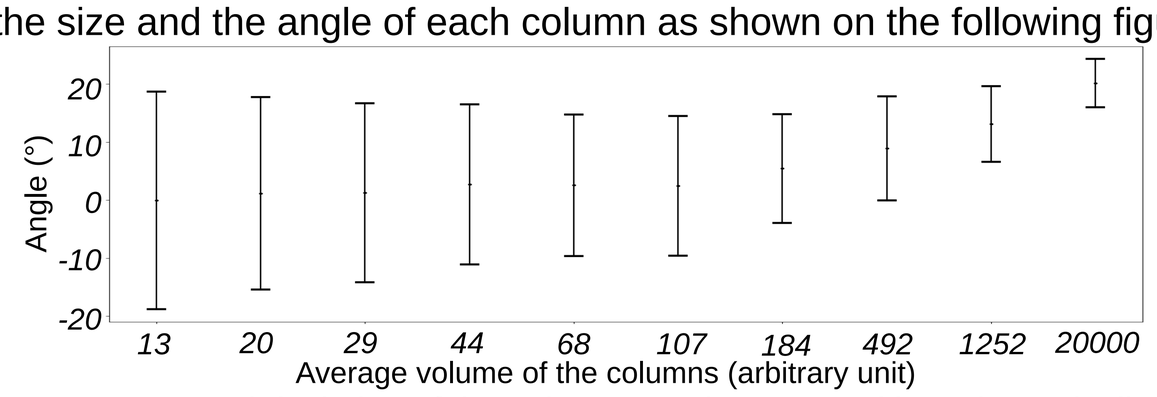
Azimuthal component of the column angle (top view)

From the column angle to the coating angle



2D SEM-like image of a simulated film with colour applied to each column

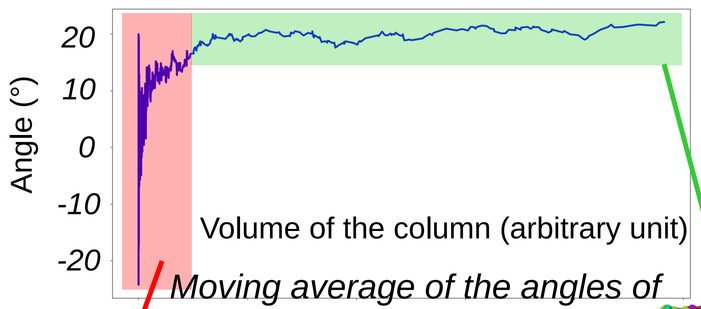
First approach: **averaging** the angle of **every columns** weighted by their respective **size** (defined by the volume in this study). With this evaluation the standard deviation approach 7° for a 30° averaged angle. A more detailed investigation highlights the dependency between the size and the angle of each column as shown on the following figure.



Average and deviation of the columns angles grouped by volume deciles

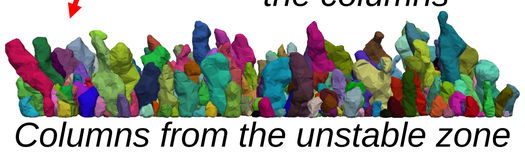
This first approach can hardly answer the need of a robust methodology.

Second approach: use the **moving average** of the column angle sorted by their **decreasing volume**.

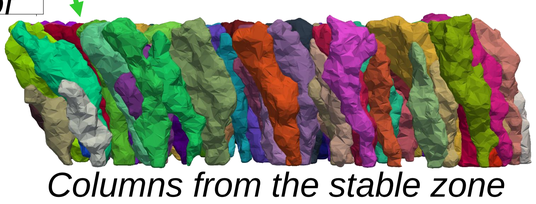


The graph shows two zones:

- unstable zone for small columns,
- stable zone for the large columns.



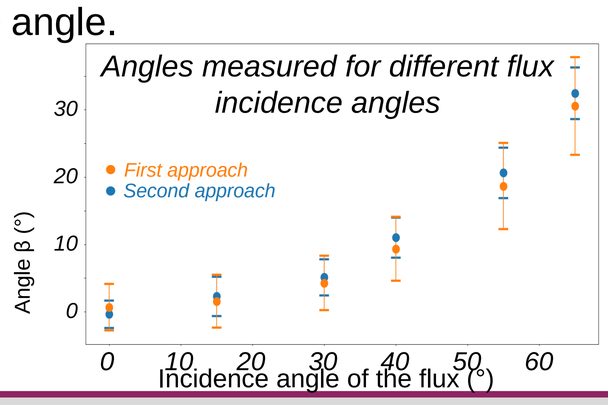
Columns from the unstable zone



Columns from the stable zone

Only the angles of the stable zone will be used for the coating angle. The threshold between the two zones is defined based of the acceptable variation of the average angle.

The measurement made according to the second approach presents lower dispersion compared to those conducted according to the first approach.



Conclusions

- This study enables the evaluation of the angle of simulated thin films in a comprehensive and robust manner.
- As measurement are conducted on every column, it is possible for specific application to have a column by column investigation.
- The threshold solution has been compared to the “naïve” solution.
- The most important contributor to the quality of the measurement is the size of the initial simulated substrate.