PWIE 06-05-2022

Study on nano-columnar tungsten under Ar irradiation

Álvaro López Cazalilla, Fredric Granberg, Kai Nordlund

Department of Physics, University of Helsinki

Collaborators

- Christian Cupak (TU Wien)
- Martina Fellinger (TU Wien)
- Paul S. Szabo (Space Sciences Laboratory, University of California)
- Andreas Mutzke (Max–Planck Institute for Plasma Physics)
- Friedrich Aumayr (TU Wien)
- Raquel González-Arrabal (UPM)

Introduction & Motivation

- Nuclear fusion as a source of energy.
- The proper choice and design of a material to withstand the extreme conditions is a bottle neck. Tungsten is the best candidate.
- The nanostructured W has shown to alleviate some of the problematic conditions in the future reactor chamber e.g erosion.
- Computational methods are powerful tools to model materials and understand these (irradiation-induced) changes

Introduction & Motivation: Simulation details

- We use molecular dynamics (MD) to study the W irradiation with Ar for different surface morphologies.

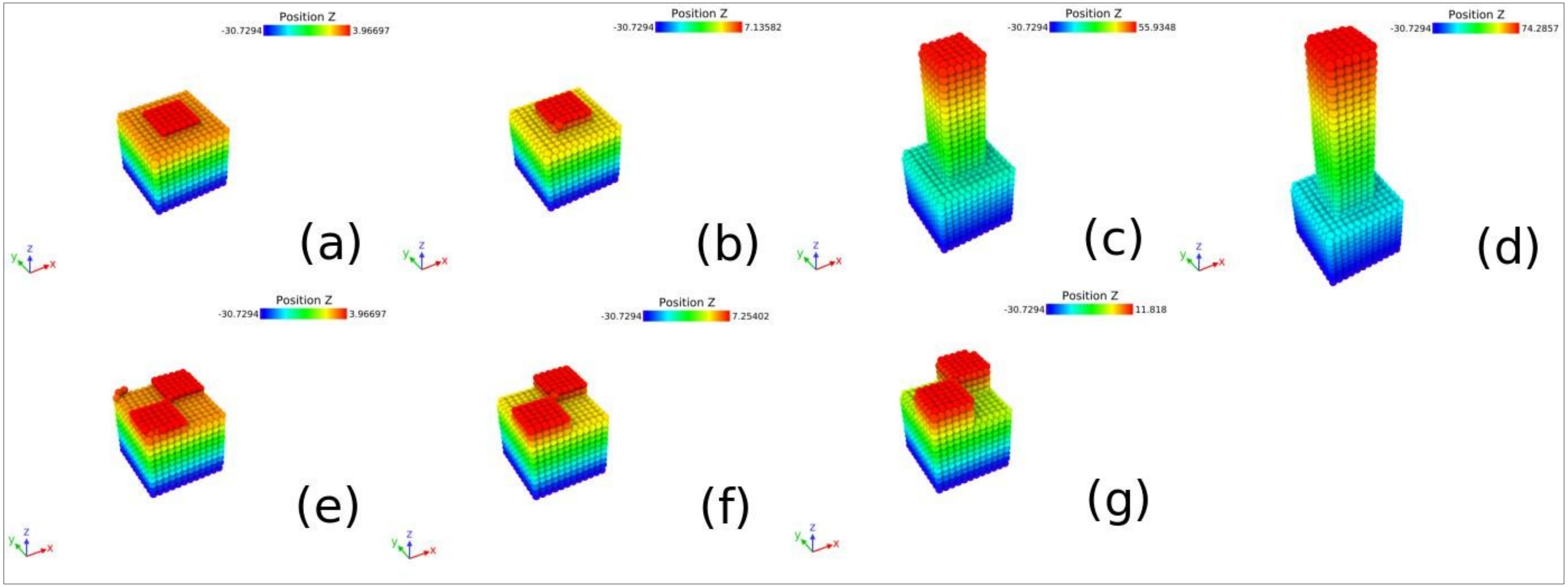
- Marinica potential for W-W interaction. Repulsive pair potential for Ar-W and Ar-Ar

- Thermal bath at the border. NVE elsewhere, the temperature is recovered to 300 K prior to next impact (sequential mode), and the bottom is fixed to prevent cell movement during the sequential irradiation (2000 Ar impacts) at several angles (0^{o}-80^{o}) for 1000 and 2000 eV. We also study the single impact case (10000 impacts) for a small simulation cell with different pillar heights (toy model) at 100 and 200 eV.

- We extract information on how many atoms fly away from the surface per impact (sputtering yield), which atoms are sputtered and how the surface changes as the fluence increases.

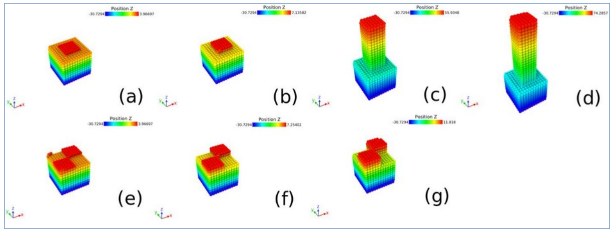
Toy model

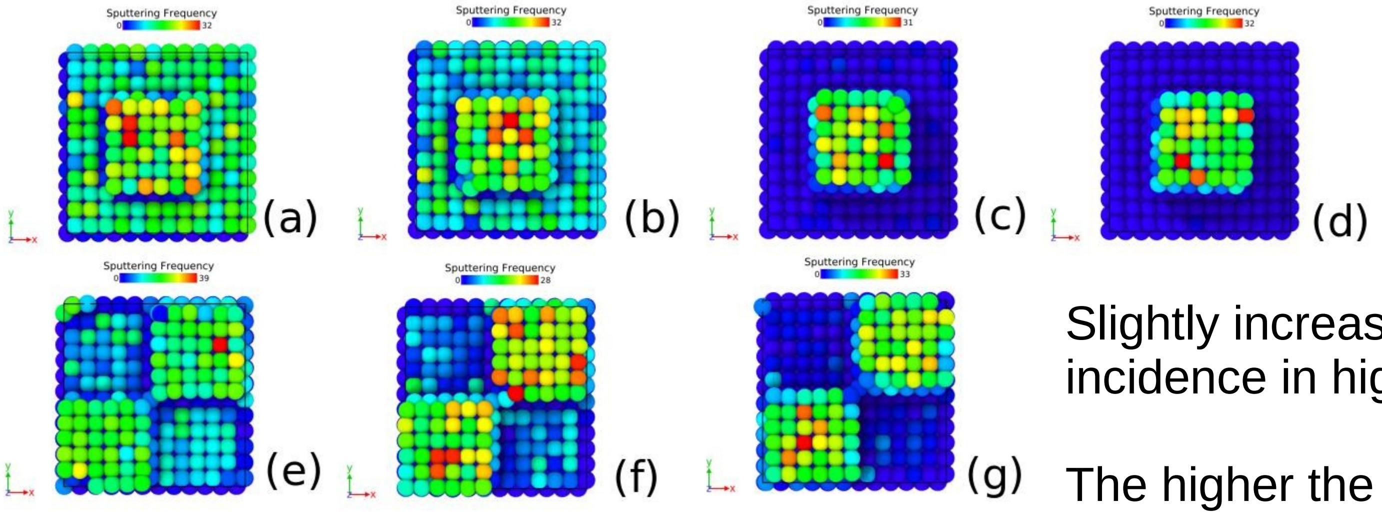
Single impact mode



- We consider different heights and covered areas
- We follow the sputtering yield and the atoms that are more frequently sputtererd
- 10000 cases for each case at 100 and 200 eV

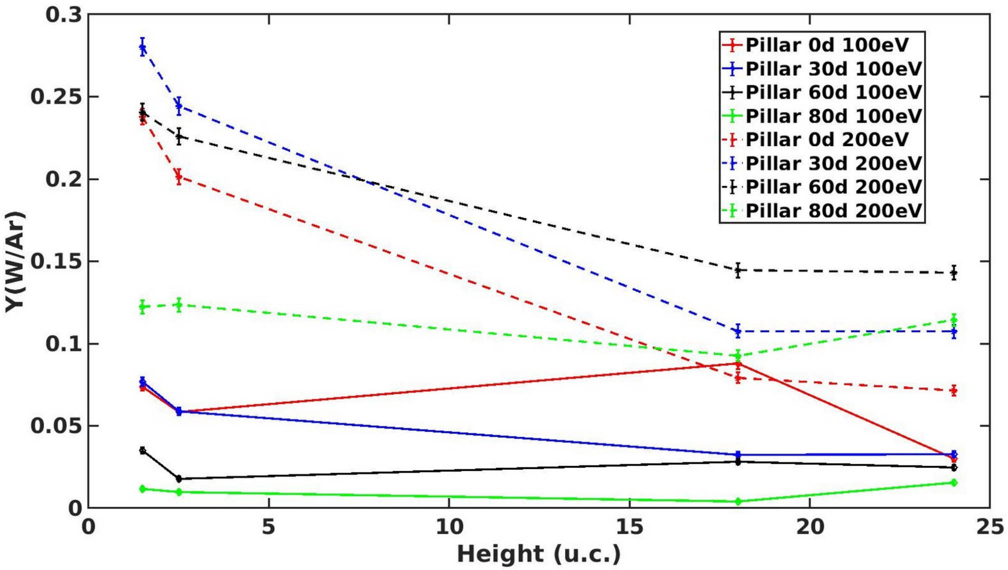
Toy model

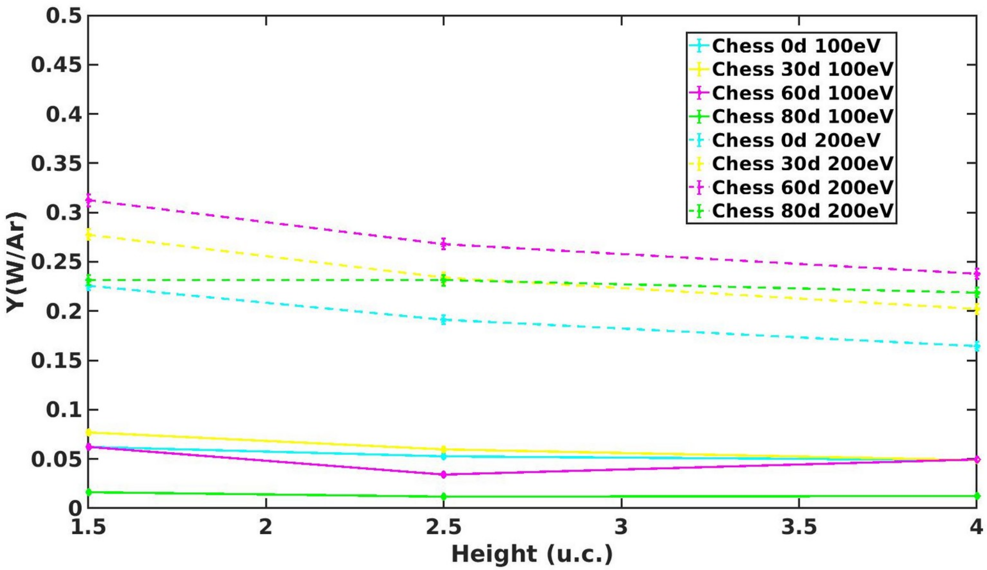




Slightly increase of sputtering at grazing incidence in higher structures

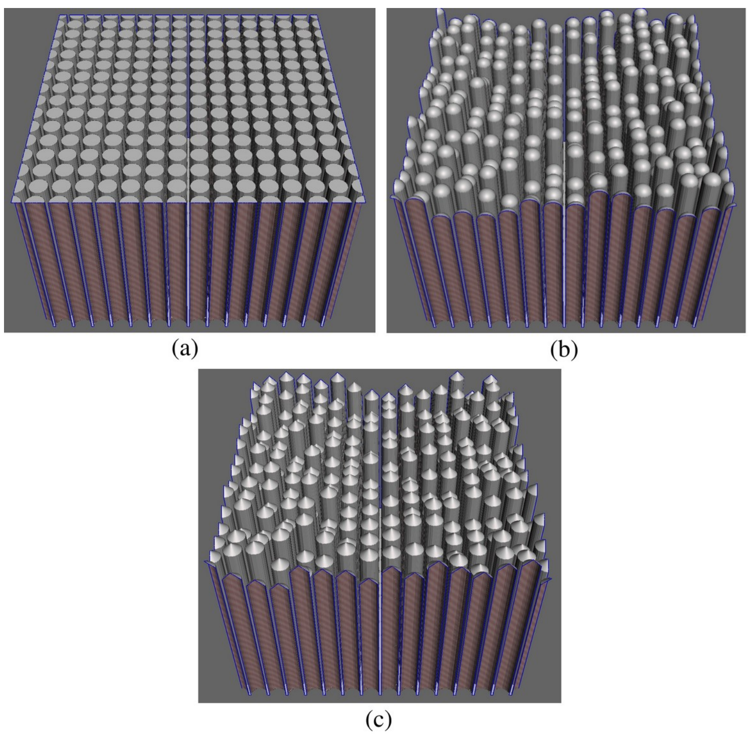
The higher the structure, the less the sputtering is in the base of the pillar(s)



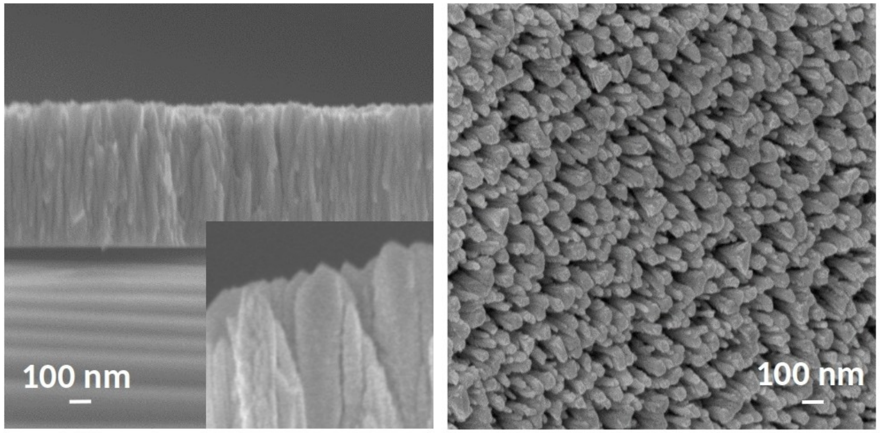


Nano-colums: Comp. with experiments

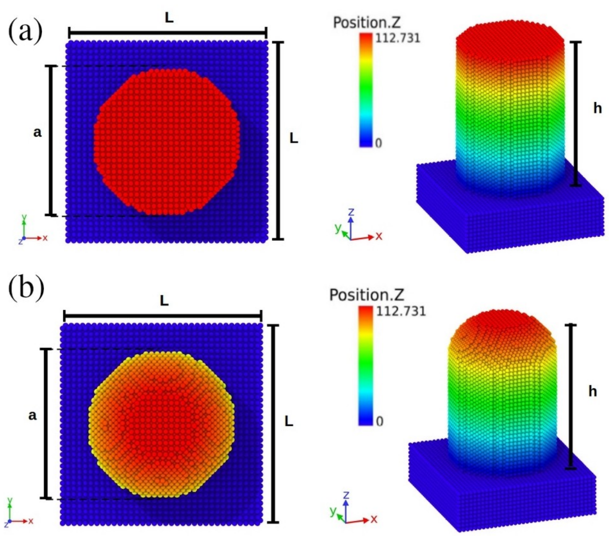
- We compare our results with SPRAY (BCA) and experiments [1], approximating the aspect ratio of the W columns



Different shapes on the tops, variation in the height



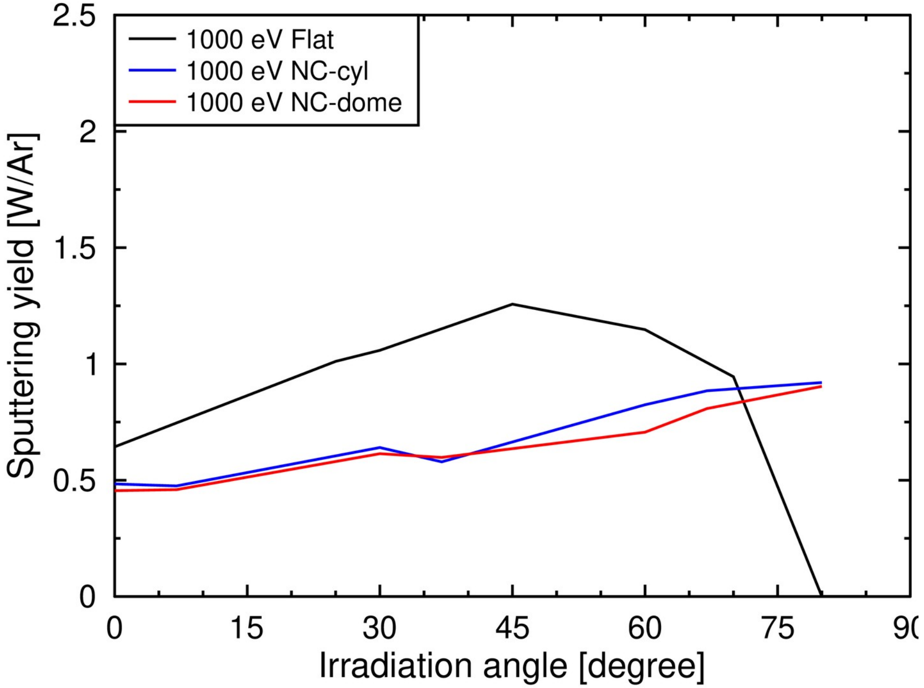
(a) (b)

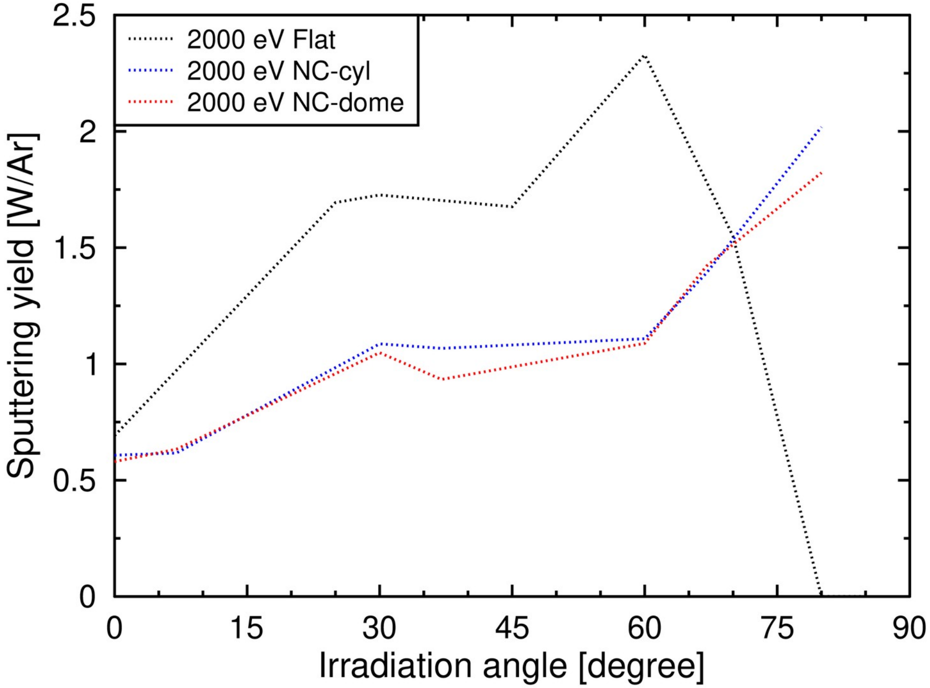


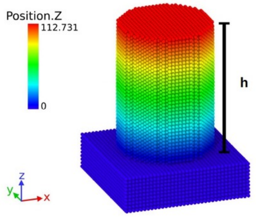
Different shapes on the tops, fixed height and aspect ratio

[1] A. Lopez-Cazalilla, C. Cupak et al., submitted (2022)

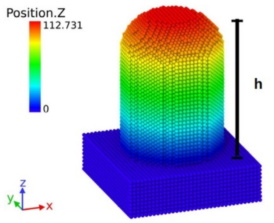
Comparison with (100) flat surface







NC-cyl

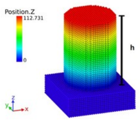


NC-dome

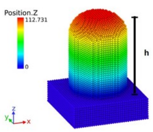
- We observe that in the flat surface, the sputtering drops at grazing incidence.
- In general, lower sputtering when the nanocolumn is included.

[1] A. Lopez-Cazalilla, C. Cupak et al., submitted (2022)

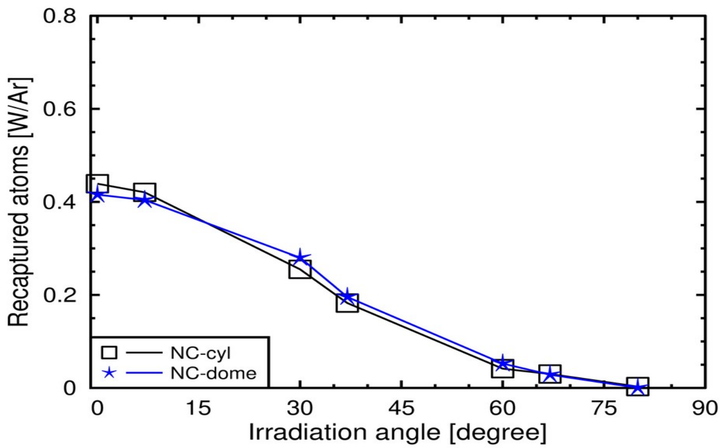
Recaptured atoms in the NC

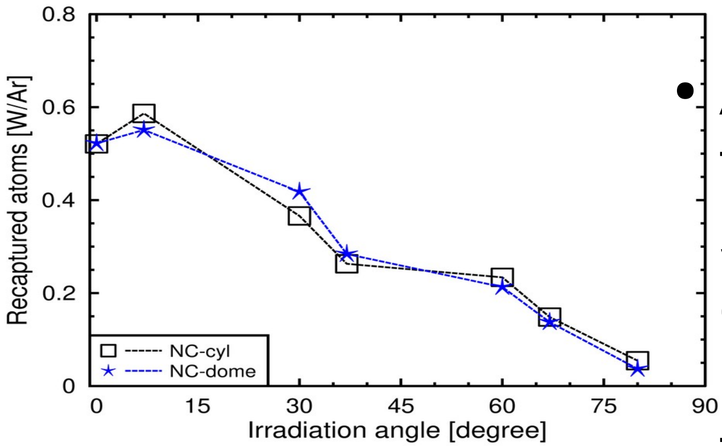


NC-cyl

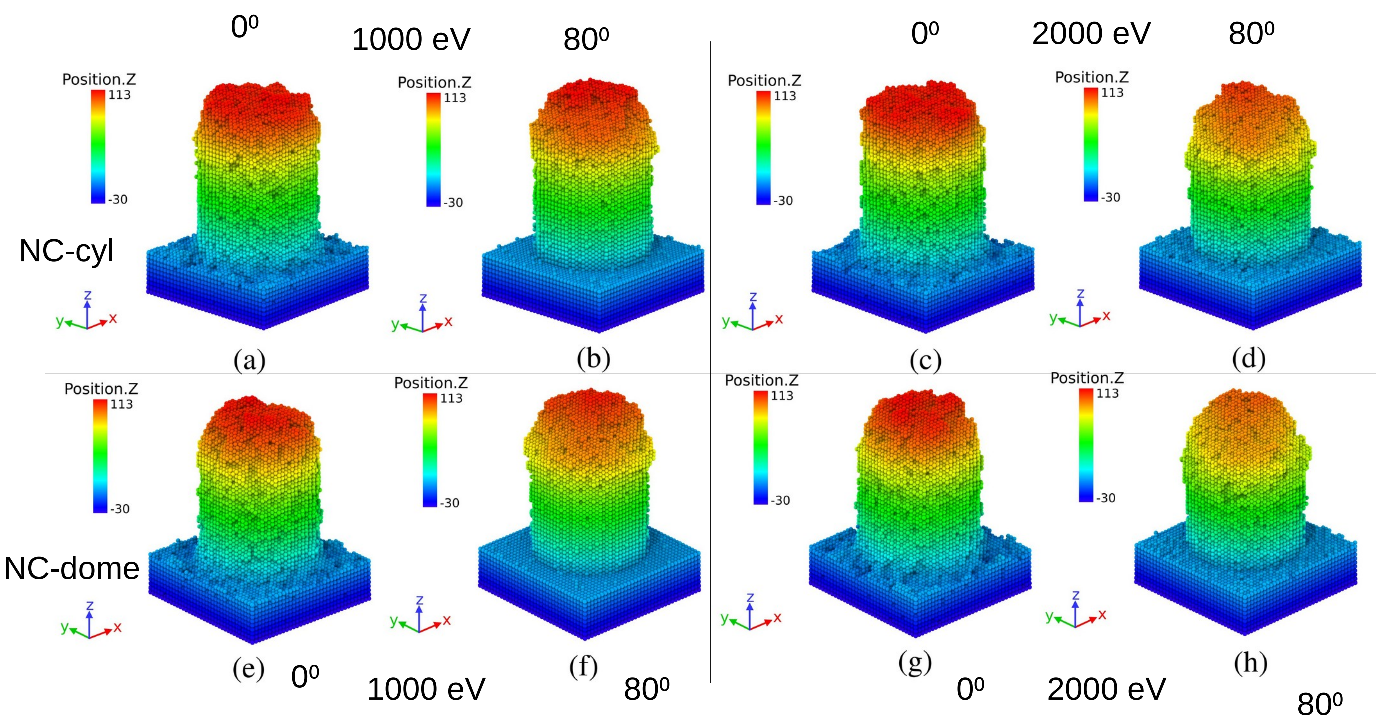


NC-dome



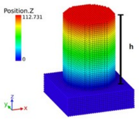


- Atoms sputtered from the bottom surface end more often in the NC at normal incidence than at grazing.
- This effect increases with the energy.
- The NC is more damaged at grazing incidence

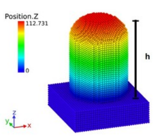


[1] A. Lopez-Cazalilla, C. Cupak et al., submitted (2022)

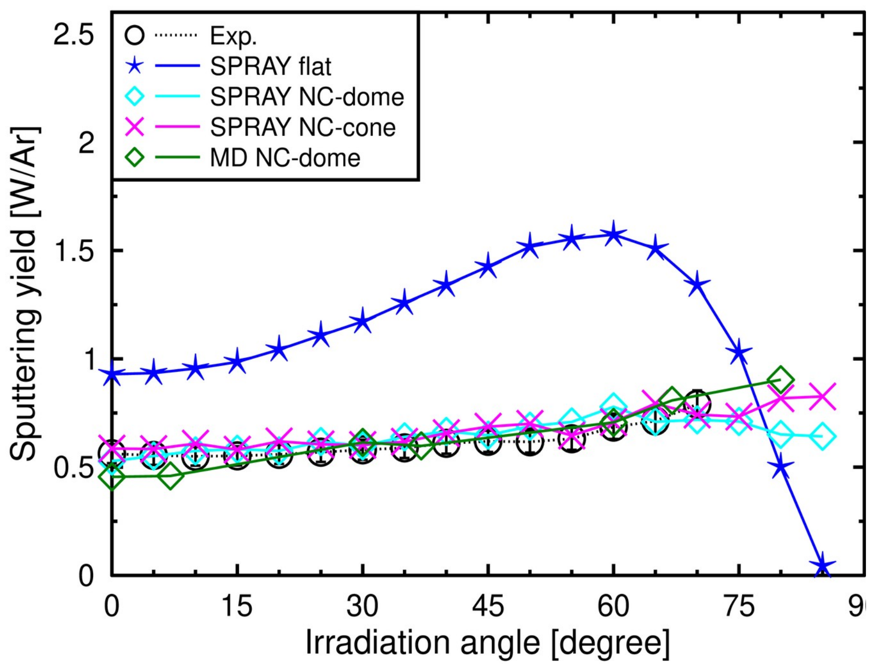
Comparison with experiments and SPRAY

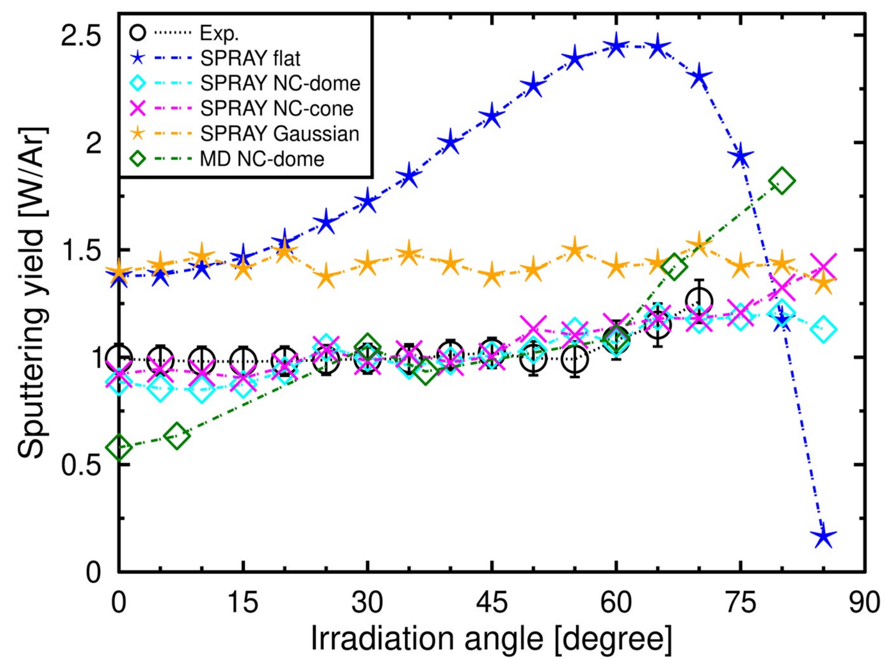


NC-cyl



NC-dome





- Good agreement at 1000 eV with both experiments and SPRAY
- Fairly good agreement with experiments at off-normal irradiation angle for 2000 eV
- MD overestimates the sputtering yield at grazing incidence compared to SPRAY

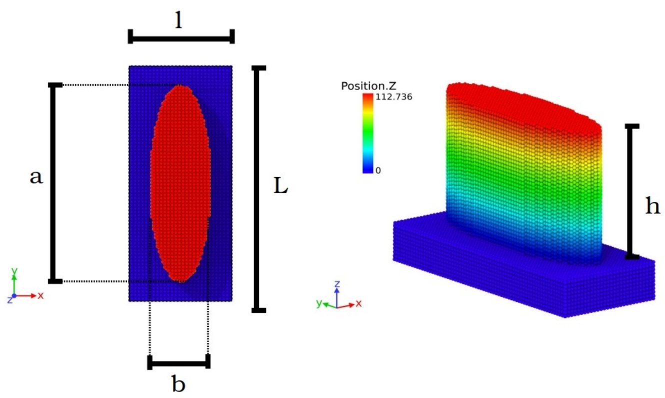
[1] A. Lopez-Cazalilla, C. Cupak et al., submitted (2022)

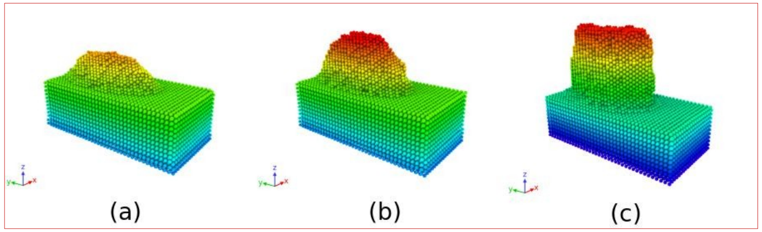
Conclusions

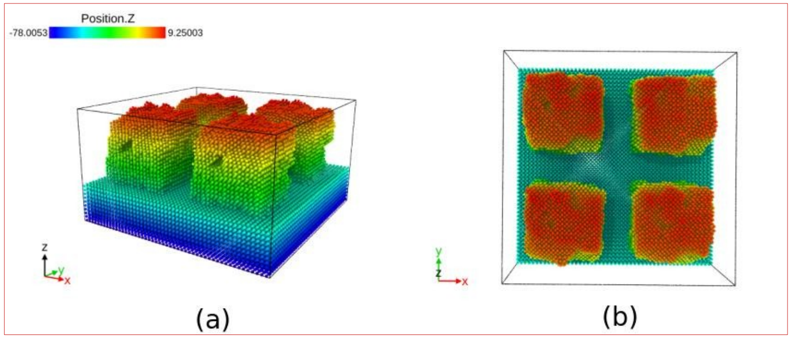
- The nanostructuring of the W surface suppresses the sputtering yield in most of the irradiation angles range.
- The toy model allows to easily see the importance of the surface coverage and the height of the pillars in order to suppress the sputtering yield
- Those atoms less coordinated are more likely to be sputtered
- The top of the NC seems to decrease the sputtering yield in the dome case compared to the flat top case. The troughs between columns play a role in reducing the sputtering yield.
- Good comparison with SPRAY and experiments.

On-going & future work

- Importance of the surface coverage and shape of the NC
- The introduction of different structures such hemi-ellipsoids or fuzzz induces change in the sputtering yield, but how much?







Thank you for your attention