Spanish Fusion HCP Workshop

Effect of surface morphology on tungsten sputtering yields

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Outline

- Motivation
- Methods
- Single-impact mode
- Sequential-impacts mode
- Conclusion & Future work

Motivation

- Nuclear Fusion is a promising source of energy
- Two different ways of plasma confinement: Inertial and Magnetic
- One of the bottle-necks for the nuclear reactors are the plama facing materials. We need to understand them in order to improve their durability.
- Computational methods can shed light on the materials study and development.
- Erosion of the surfaces, and also the formation of other structures due to irradiation (fuzz,rough,smooth) are crucial to prevent undesired effects.

Methods

- We use molecular dynamics (MD) to study the W irradiation under different circumstances (PARCAS)

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

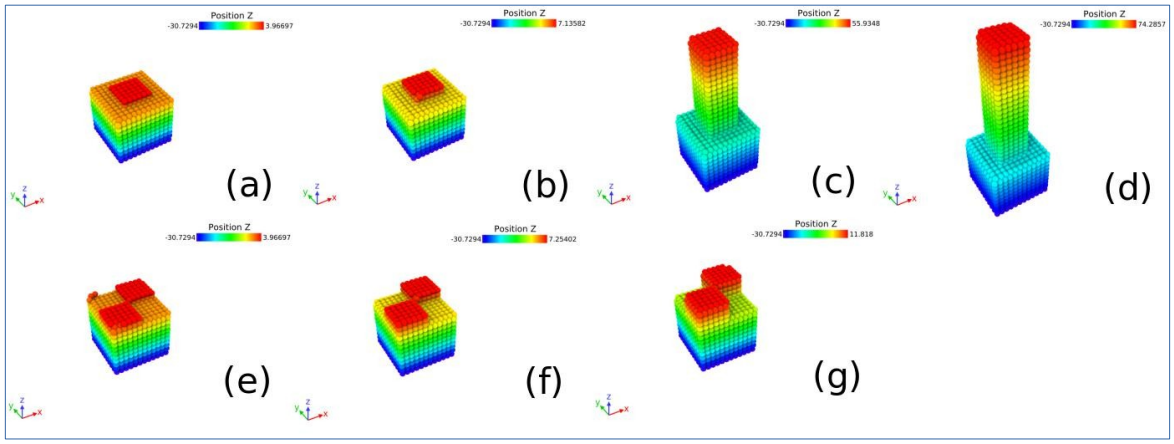
- Thermal bath in the border. NVE elsewhere, the temperature is recovered to 300 K prior to next impact (sequential mode), and the bottom is fixed to prevent cell movement.

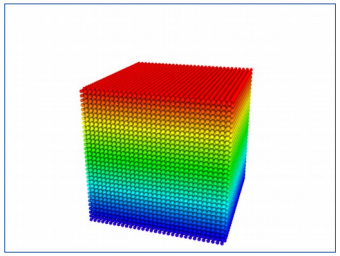
- (100) surface orientation,
  - ➔ A spinoidal decomposition to create a foam structure with porosity = 0.5.

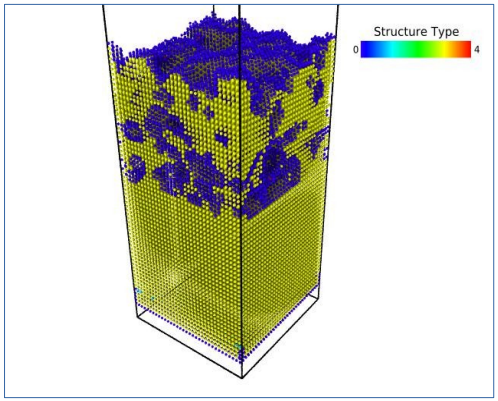
- We extract information on how many atoms fly away from the surface per impact (sputtering yield), which atoms are sputtered and how the surface changes as the fluence increases.

Methods

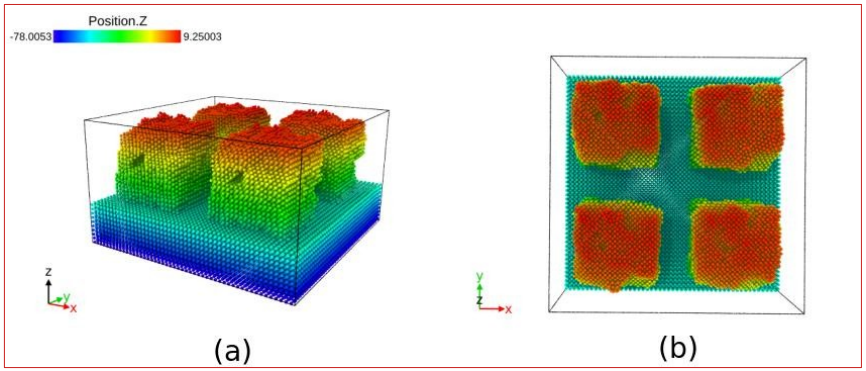
Single impact mode: cell randomly shifted, and repetition of one only event



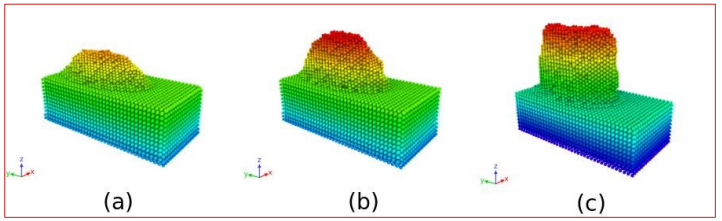


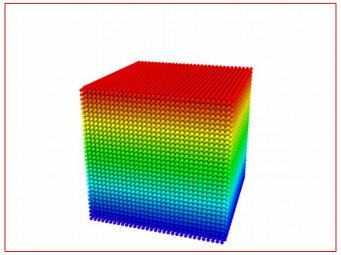


Sequential impact mode: many consecutive impacts randomly located



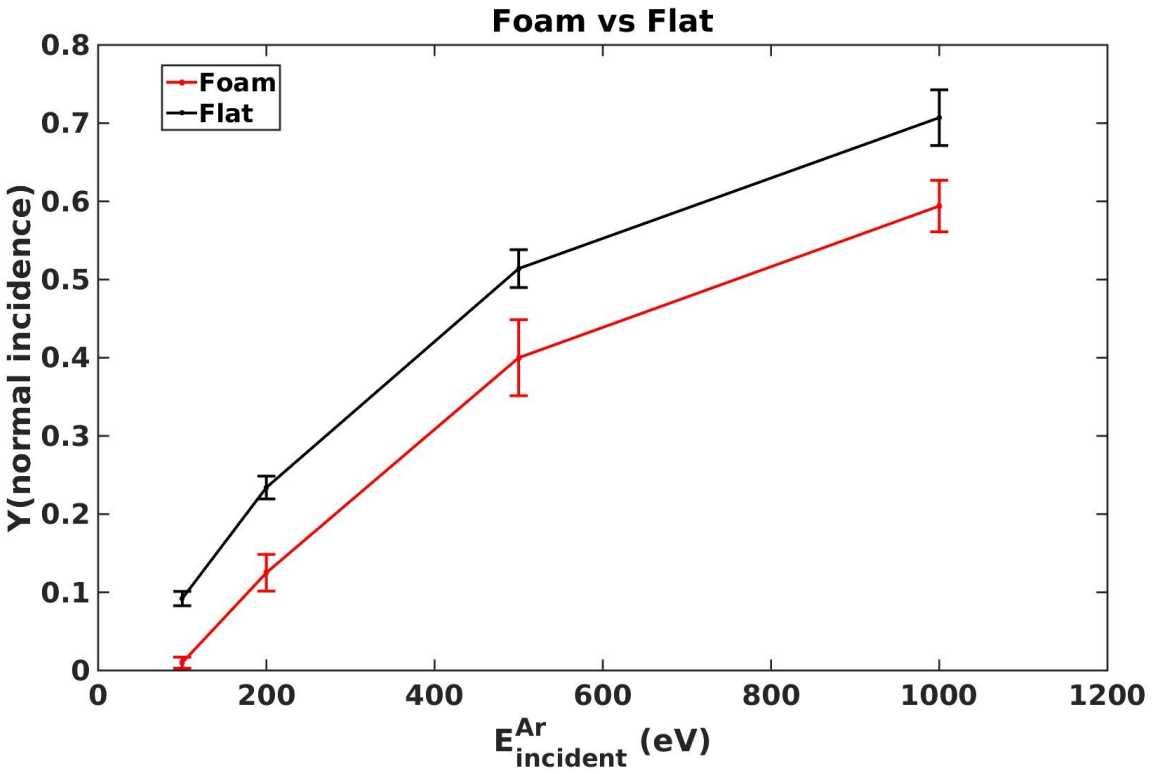
Different modes, different morphology →
Different conclusions

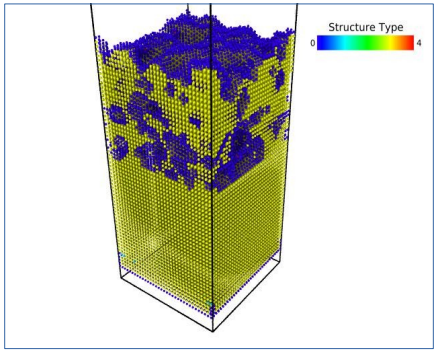


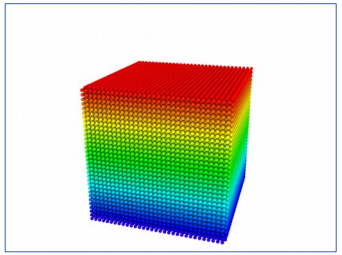


Single-impact mode

- Normal incidence (1200,5000 cases)
- Same trend
- The fuzz (foam) acts capturing some W atoms that could be eroded since the surface is not flat.

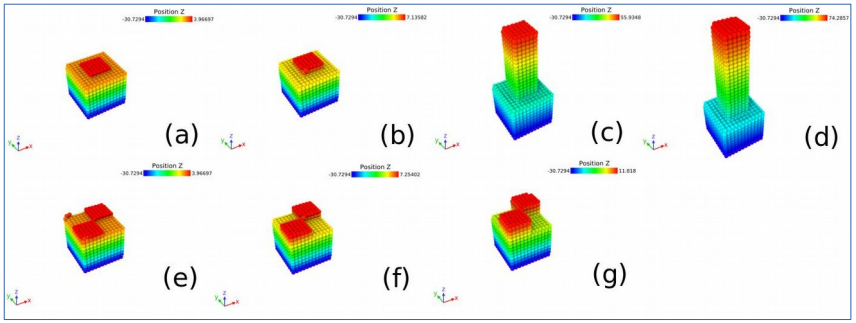


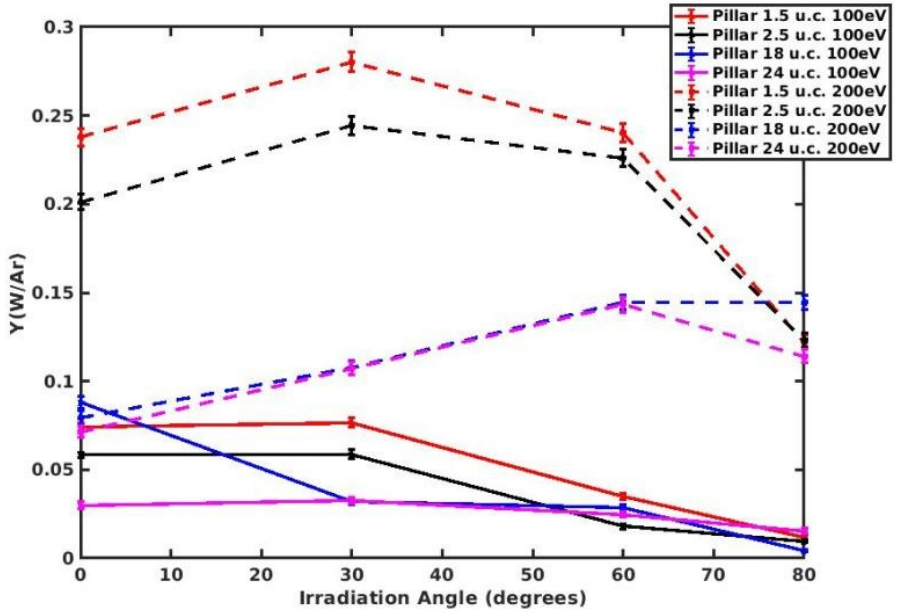




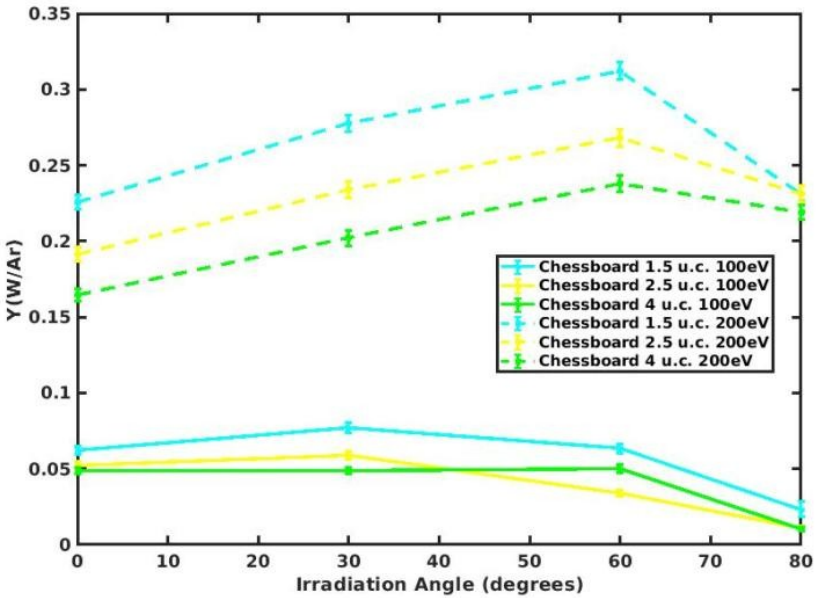
Single-impact mode

- 10000 cases for each case at 100 and 200 eV
- In general, the higher the structure, the lower the sputtering
- Importance of the position where the atoms are sputtered from



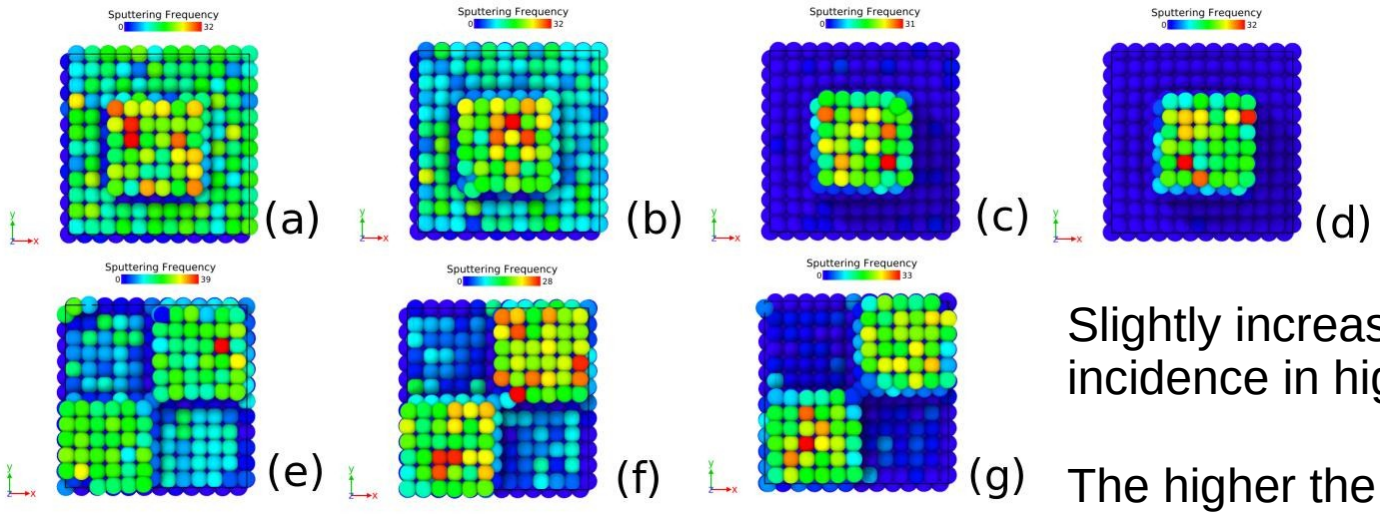


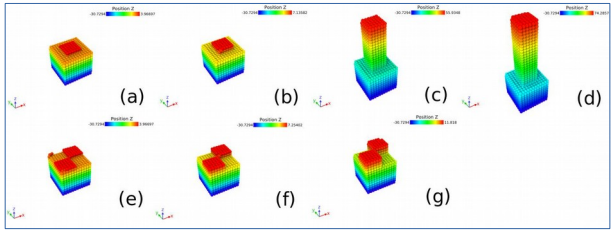
(a)



(b)

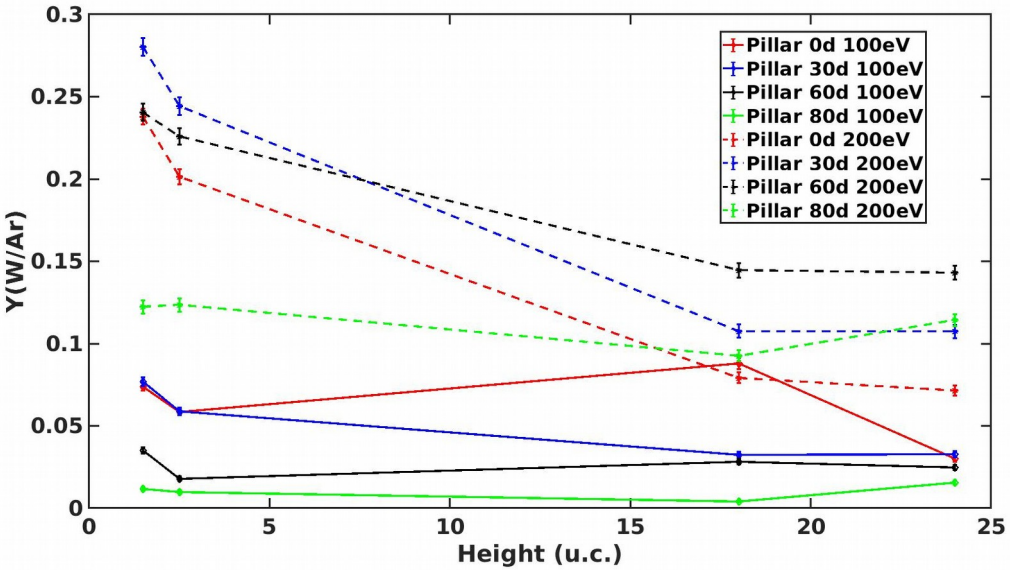
Single-impact mode

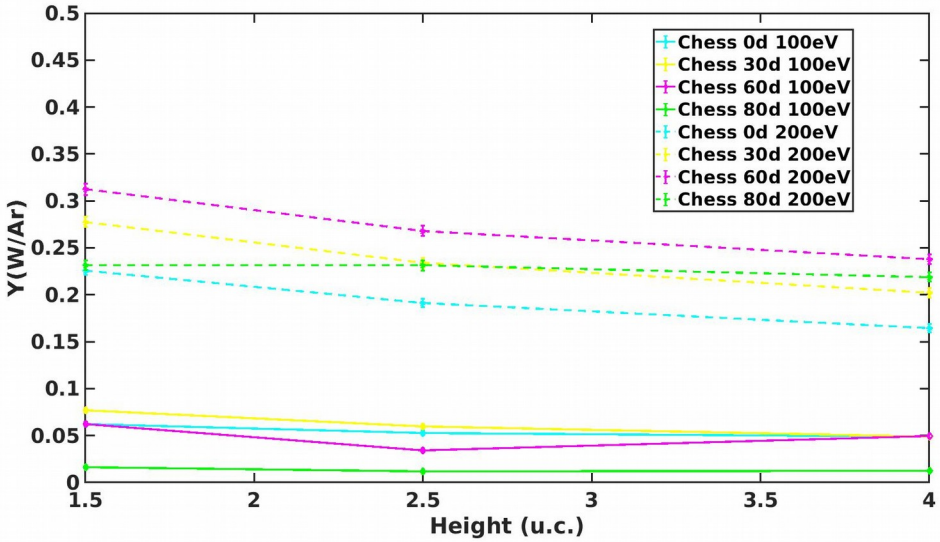




Slightly increase of sputtering at grazing incidence in higher structures

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



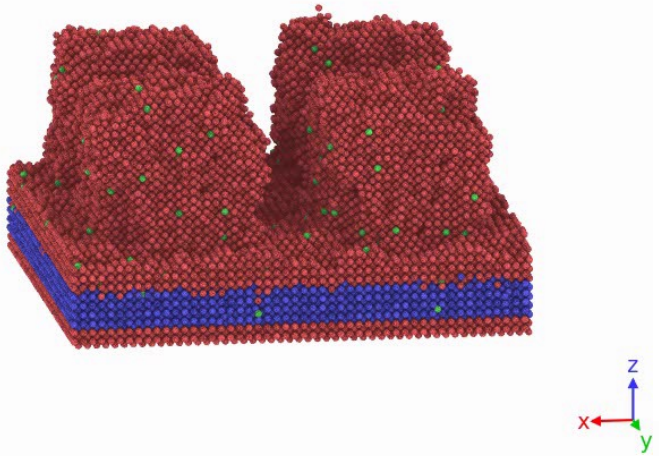


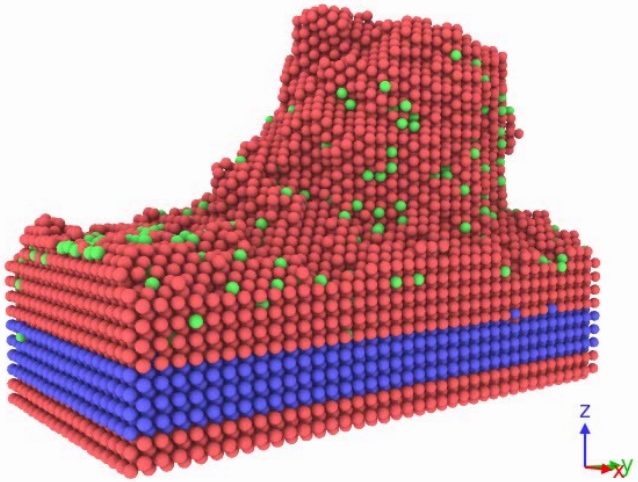
Sequential impacts mode

Fuzz – 2000 eV

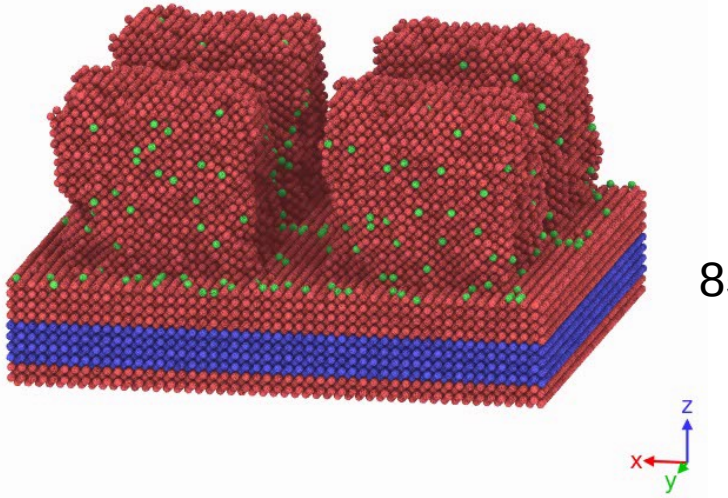
Hemispherical – 1000 eV

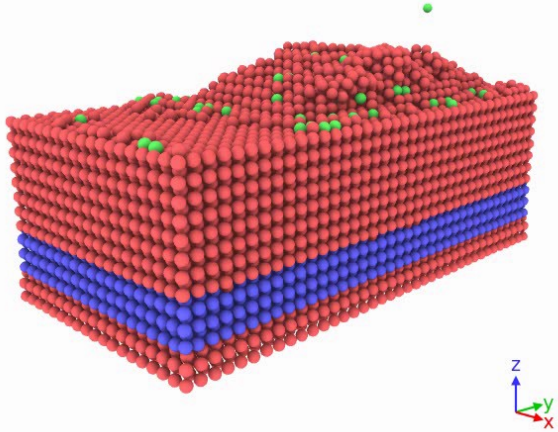
60 degrees



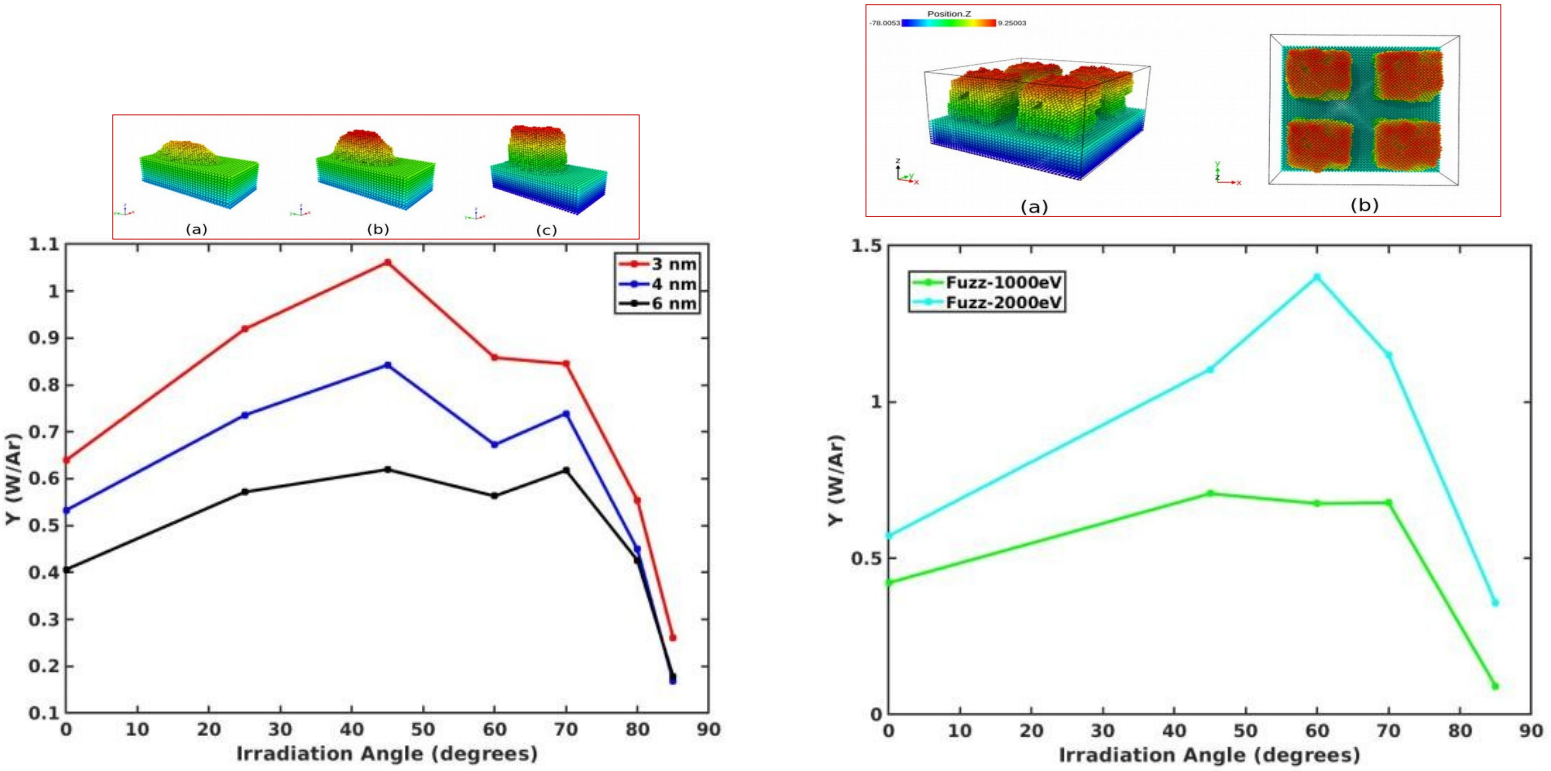


85degrees



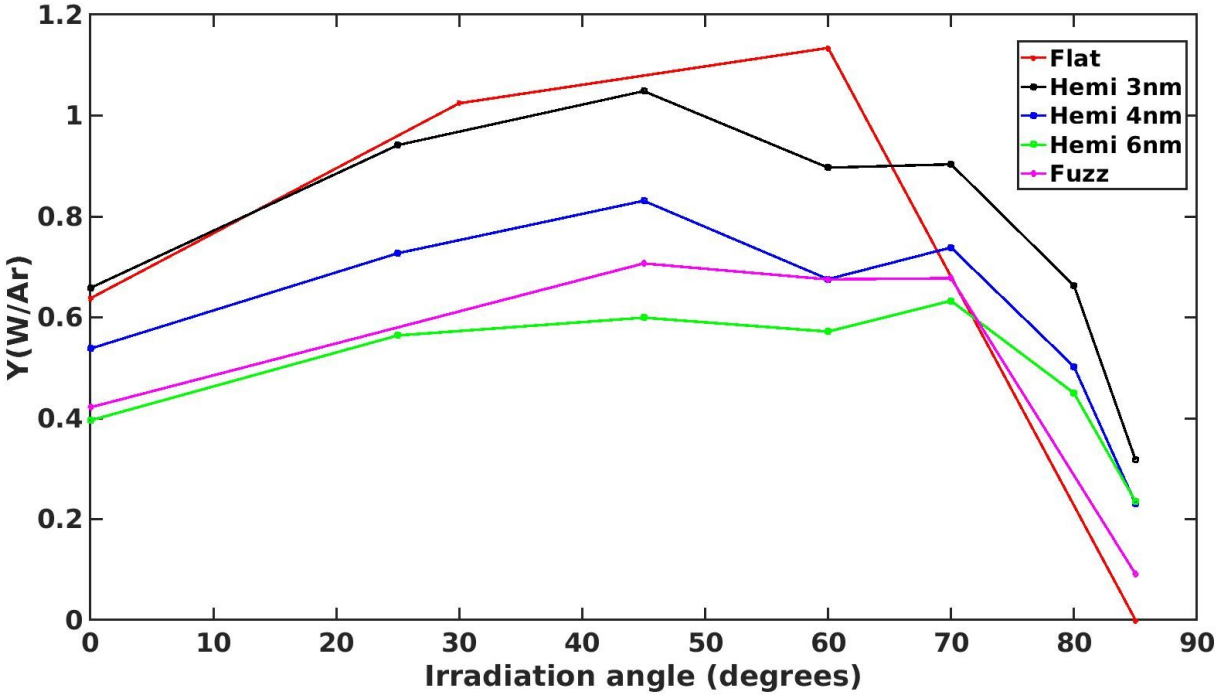


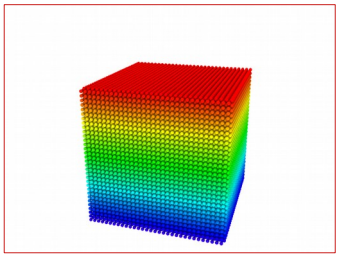
Sequential impacts mode

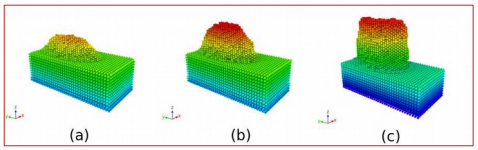


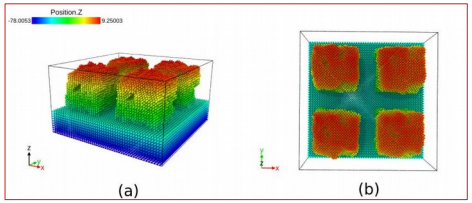
- Maximum a 45^{o} for hemisphere (3,4 nm) and 70^{o} for 6 nm after 5000 impacts at 1000 eV
- Fuzz: 1000 eV – 45^{o}, 2000 eV – 60^{o}

Sequential impacts mode









- For the flat surface, the sputtering is higher until 60^{o}
- At grazing incidence, the roughness enhances the erosion
- We observe that the fuzz increases the retention of Ar

Conclusions & Future work

- The single impact study:
  - The height of the structures (pillars) plays an important role on the erosion
  - At this level, we notice that the higher the pillars are, the surface remains almost intact
  - Those atoms less coordinated are more likely to be sputtered
  - The surface morphology of the fuzz decreases the sputtering yield
- The sequential impacts study:
  - We can obtain a more detailed evolution of different morphologies
  - The change of the morphology shows in general a lower erosion.
  - The fuzz captures more Ar ions and also some sputtered atoms from below the initial surface
- Future work: a more detailed study on different heights, more energies. Compare to experiments.

Thank you for your attention

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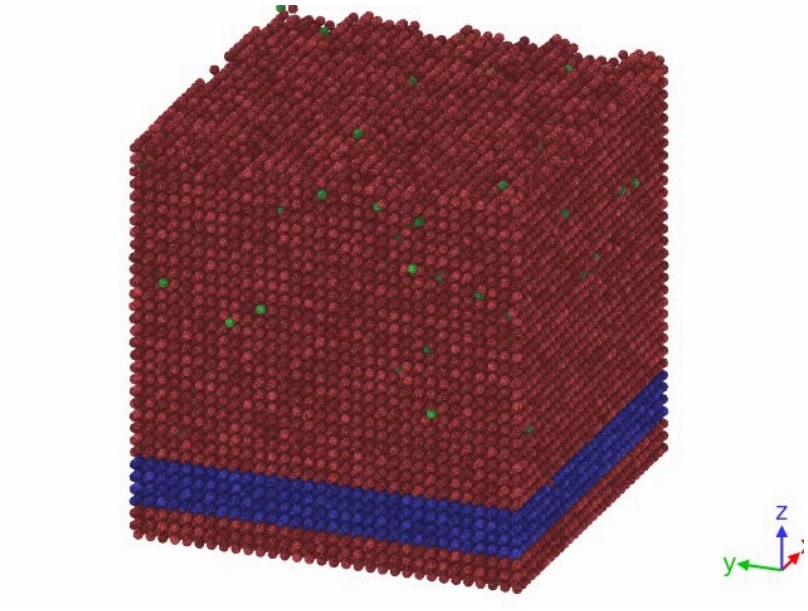
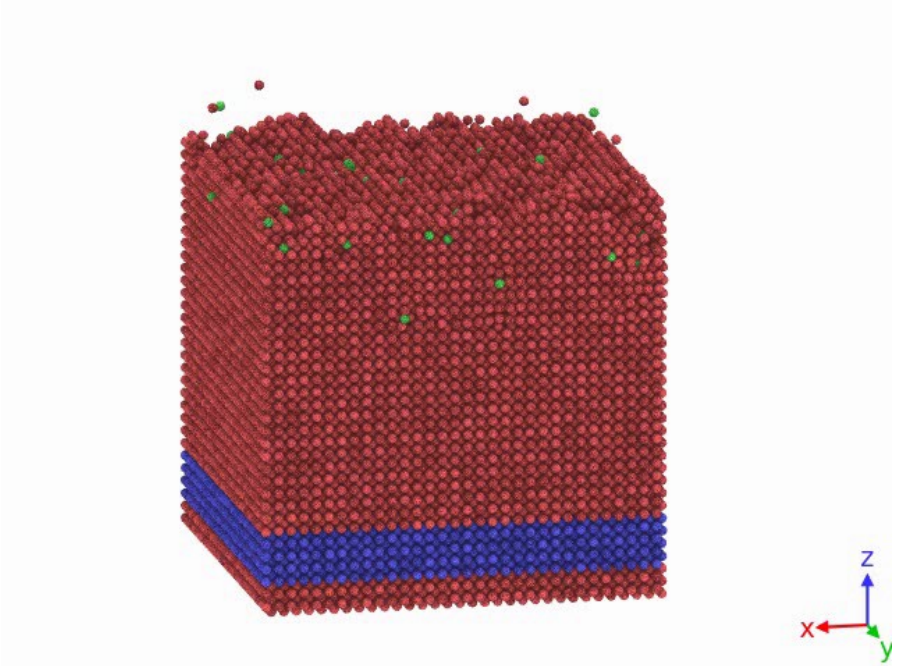
Sequential impacts

Flat surface – 1000 eV

0 degrees



60 degrees