WP-PWIE Review meeting

Development of interatomic potentials for W-B and W-O-H, and sputtering of complex surfaces

Univ. Helsinki

Fredric Granberg
Faith Kporha
Alexandre Bergero
Jesper Byggmästar
Kai Nordlund

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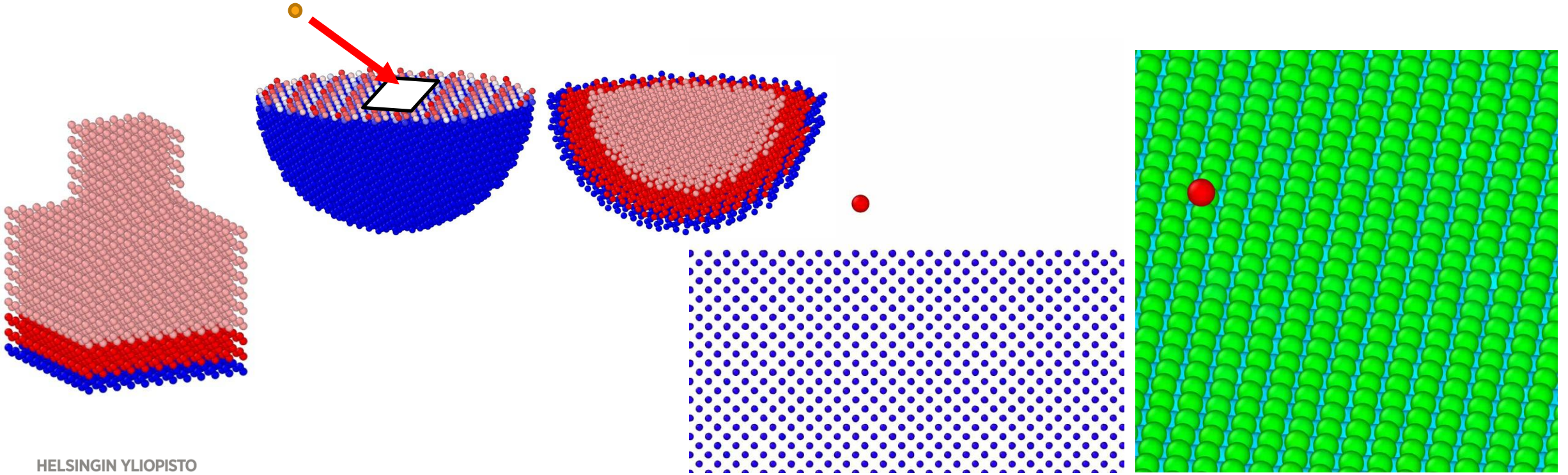
- Development of interatomic potential
  - W-B systems
  - W-O-H systems
- Sputtering of W-H surfaces
- Sputtering of HEAs
- Sputtering of W-B

Methods

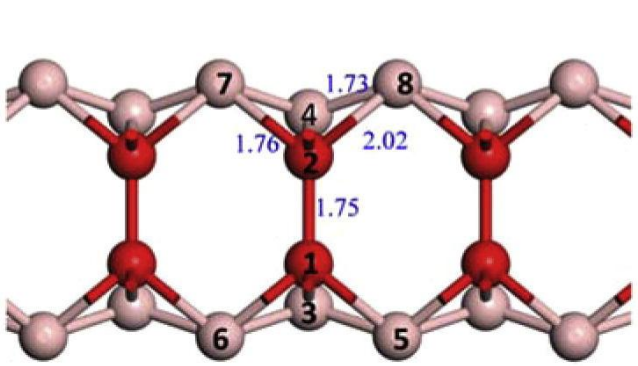
- Molecular Dynamics with classical and ML potentials



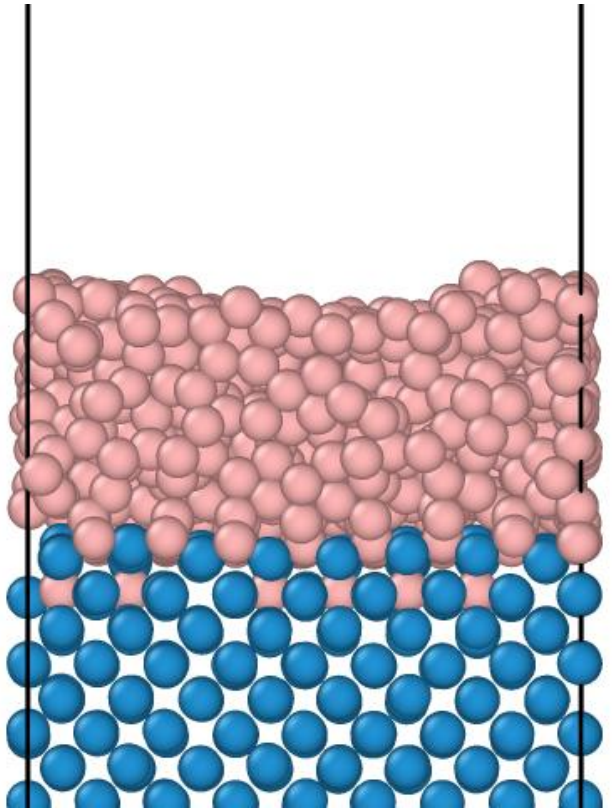
Development of W-B ML interatomic potential

- A finished W-B ML potential has been developed and tested
- Great surface properties, elastic moduli and thermal stability
- Initial sputtering and B deposition simulations successfully done
- Growth of a few layers of borophene seen for certain W surface orientations

Borophene, one of many

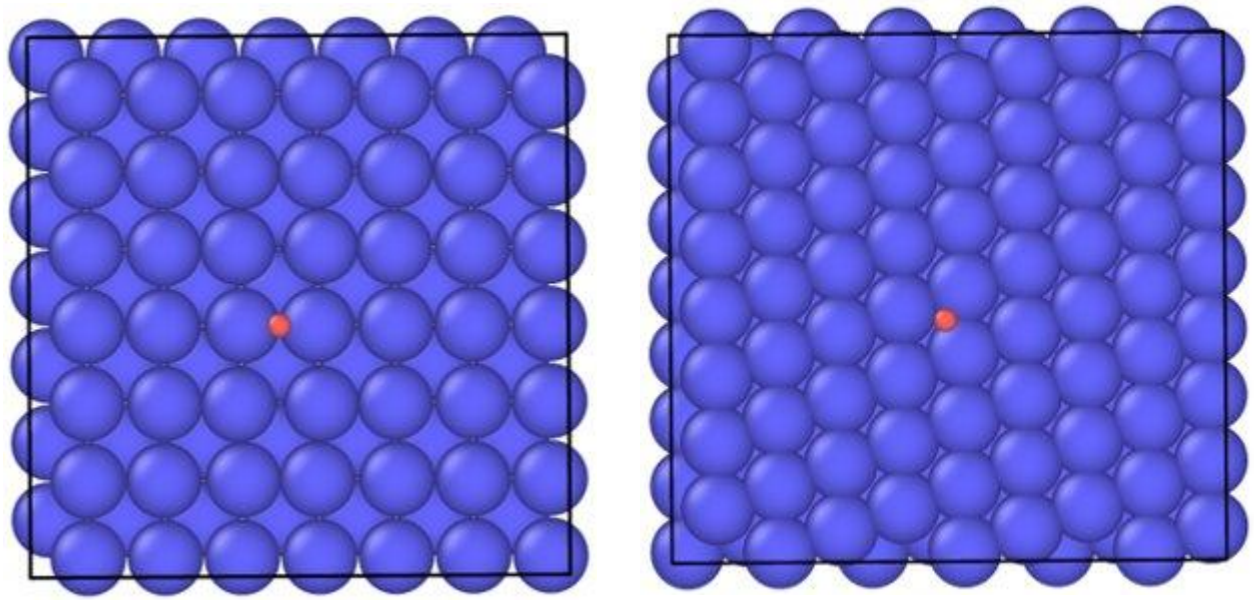


https://doi.org/10.1016/j.flatc.2017.08.008



Development of W-O-H interatomic potential

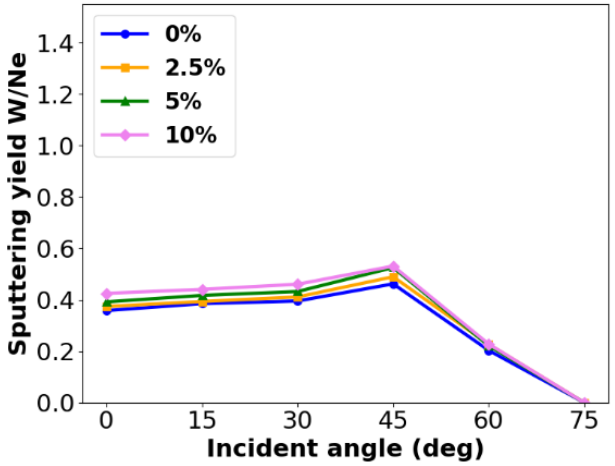
- Defect energetics good
- Correct positions of impurities as predicted by DFT
- Sputtering thresholds OK, some still inconsistent
- Some of the complex energetics missing for the O-H clusters



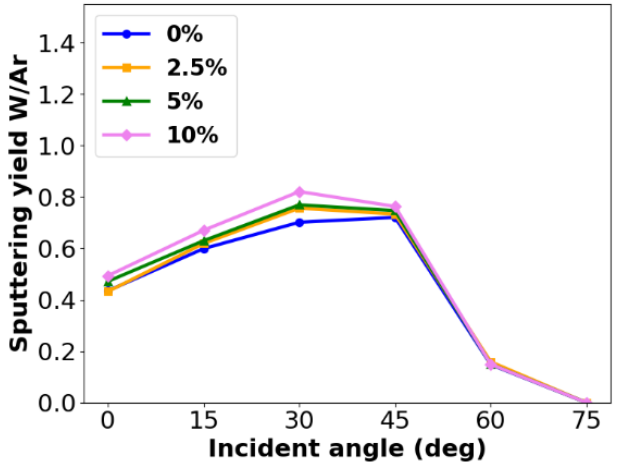
100 110

Sputtering of D-decorated W surfaces

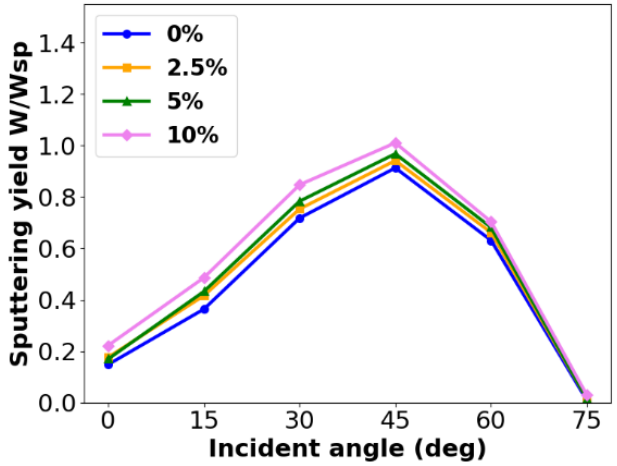
200 eV / (100) surface



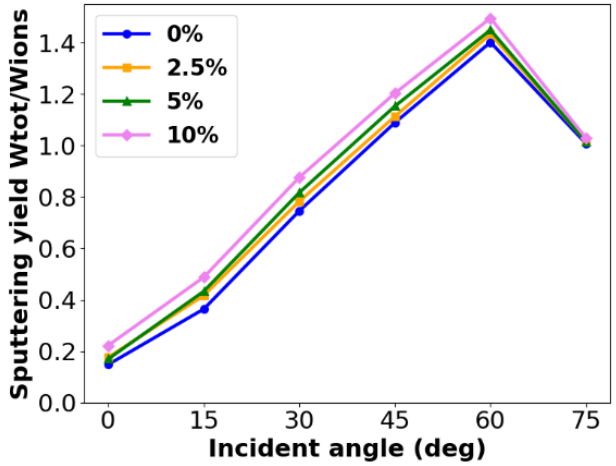
(a) Ne



(b) Ar



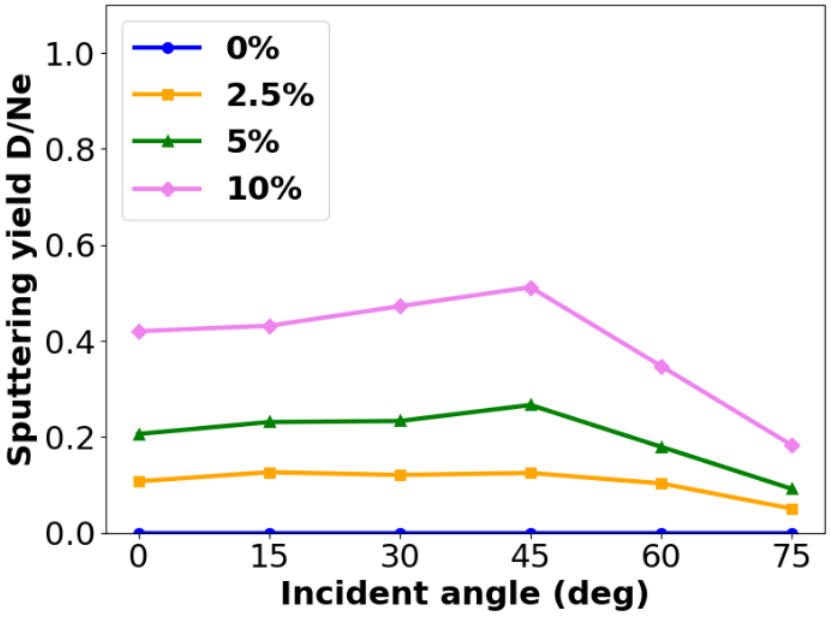
(c) W_{sp}



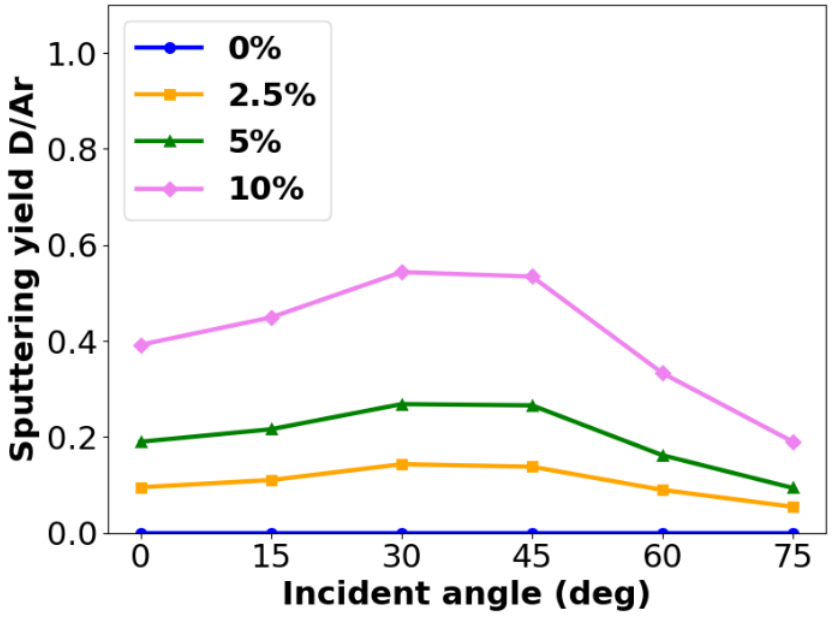
(d) W_{tot}

Sputtering of D-decorated W surfaces

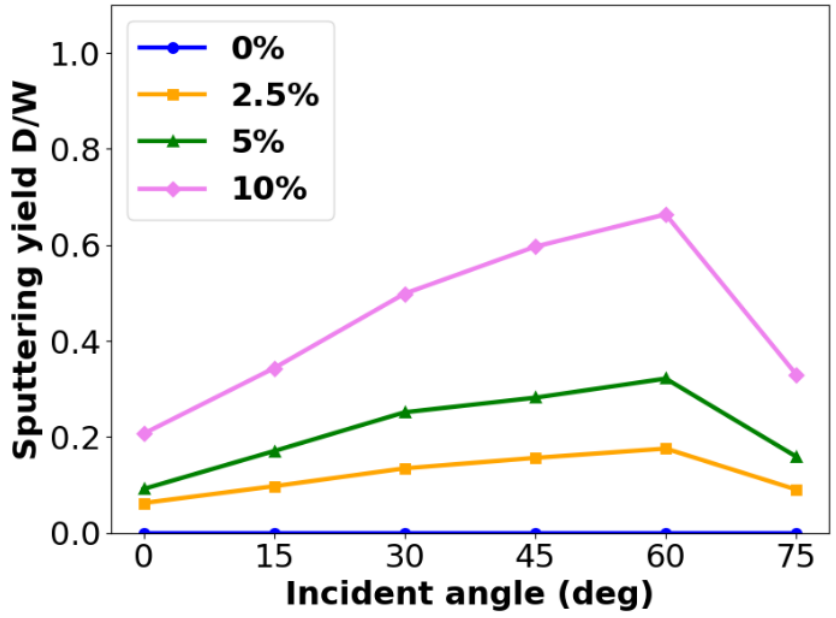
200 eV / (100) surface



(a) Ne



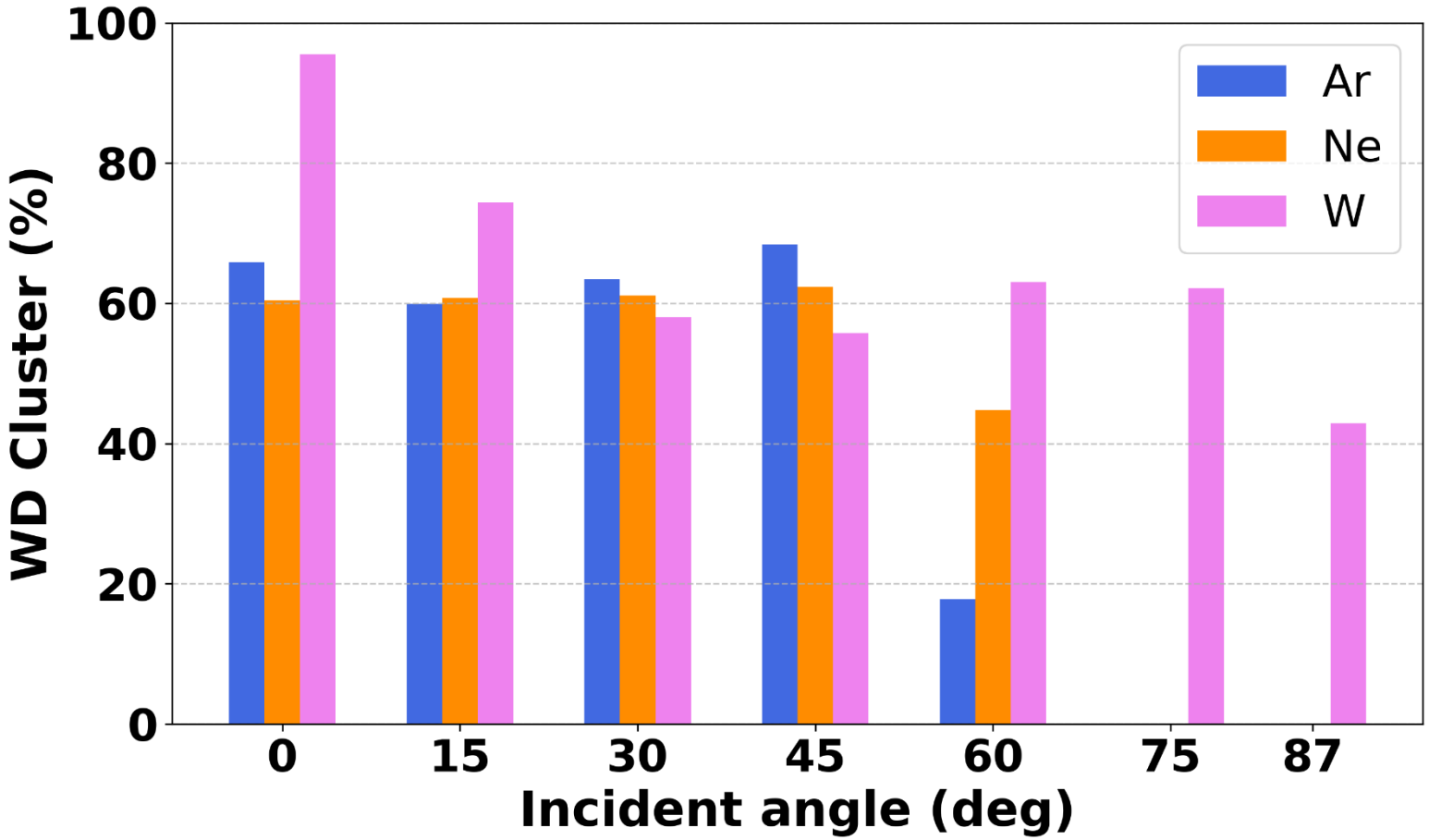
(b) Ar



(c) W

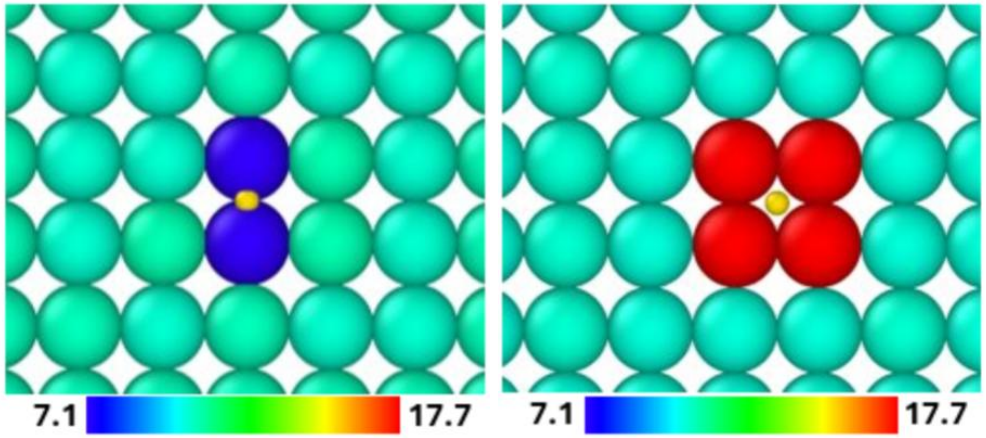
Sputtering of D-decorated W surfaces

- Average percentage of WD clusters relative to the total number of W particles leaving the surface for 10at-% D decoration
- 100 eV, average over 4 surface orientations (100,110,111 and 112)



Sputtering of D-decorated W surfaces

- We got validation of which classical potential is comparable to DFT, as previously we got opposite trends of deuterium decoration effect on the sputtering
  - It seems that deuterium decoration will increase slightly the sputtering of W
  - The D will weaken the bonds and reduce the sputtering threshold energy



(a) Mason et al. (b) Li et al.

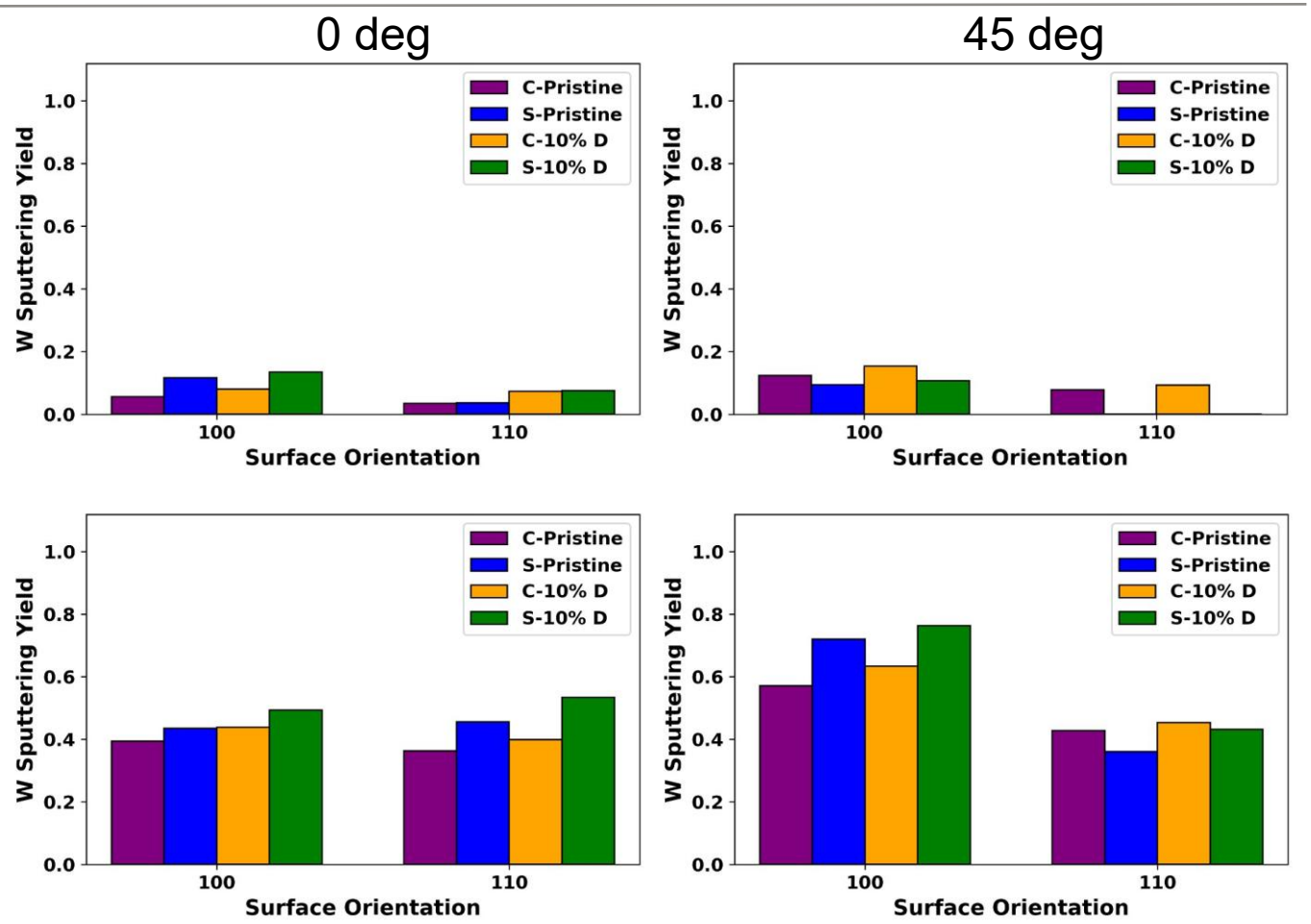
Energy required for sputtering (eV)
Both above and below figure/table

Surface	(1 1 0)				(1 0 0)			
	Spin polarized	Non-spin polarized	Mason et al.	Li et al	Spin polarized	Non-spin polarized	Mason et al.	Li et al
Pristine	11-12 eV	13.5-14 eV	12.4 eV	12.4-12.5 eV	13-14 eV	14-15 eV	10.6 eV	10.5-10.6 eV
D present	10-11 eV	13.5-14 eV	9.0-9.1 eV	16.3-16.8 eV	11-12 eV	14-15 eV	7.1 eV	17.7 eV

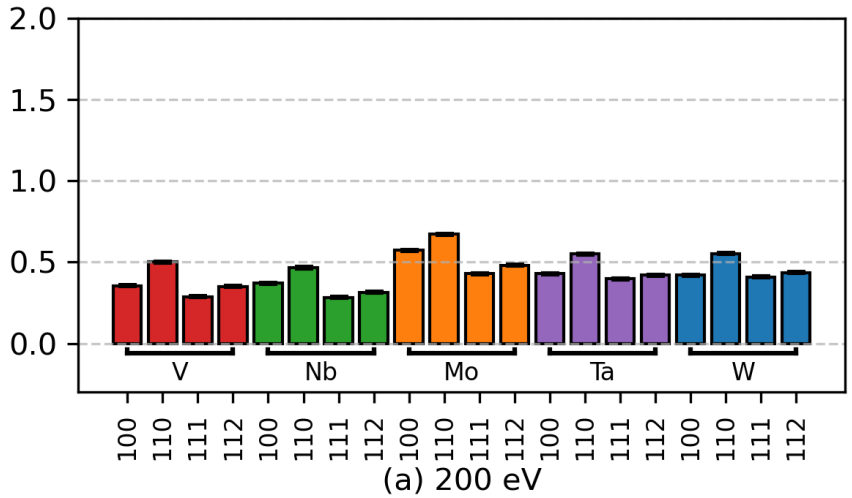
Sputtering of D-decorated W surfaces

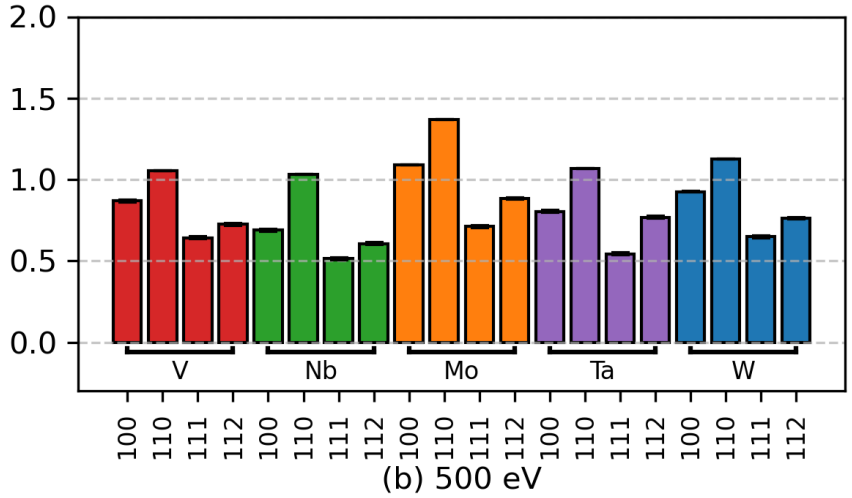
S = single impact
C = cumulative impact

Cumulative simulations essential, for instance 45 deg and 100eV

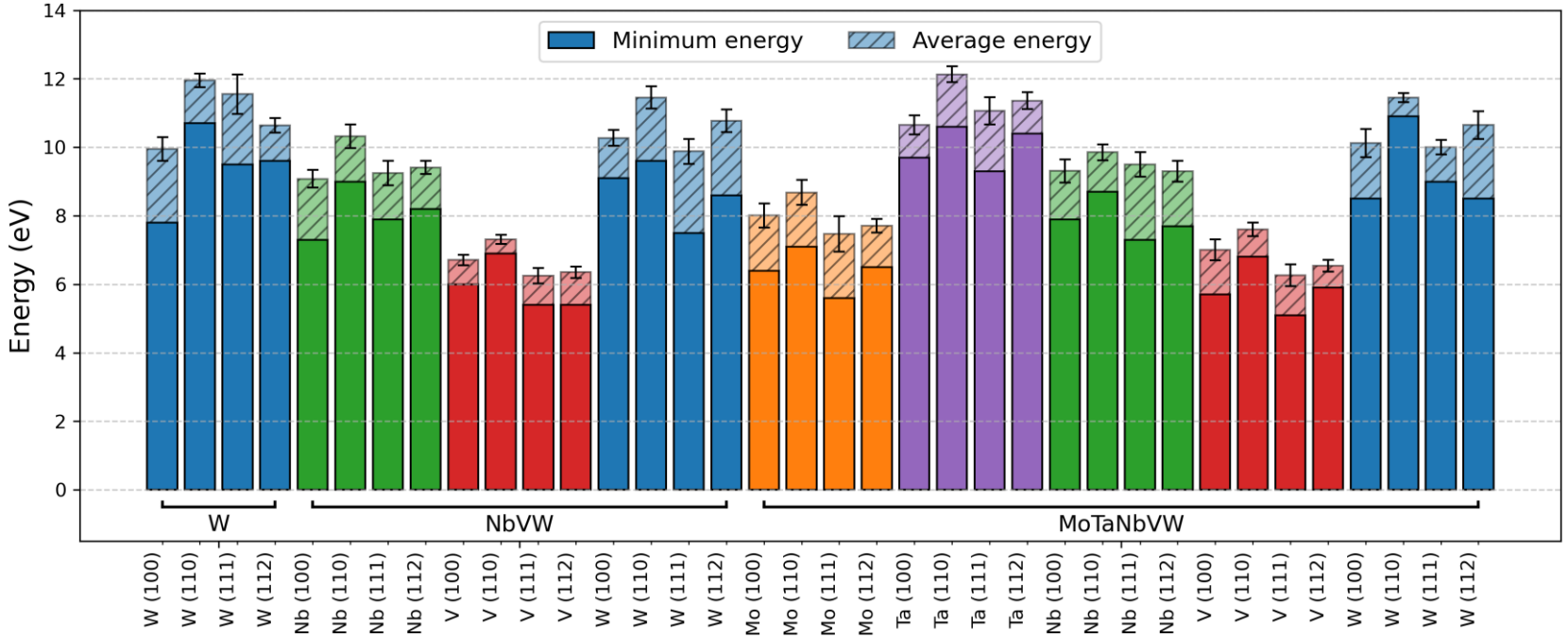


Sputtering of HEAs



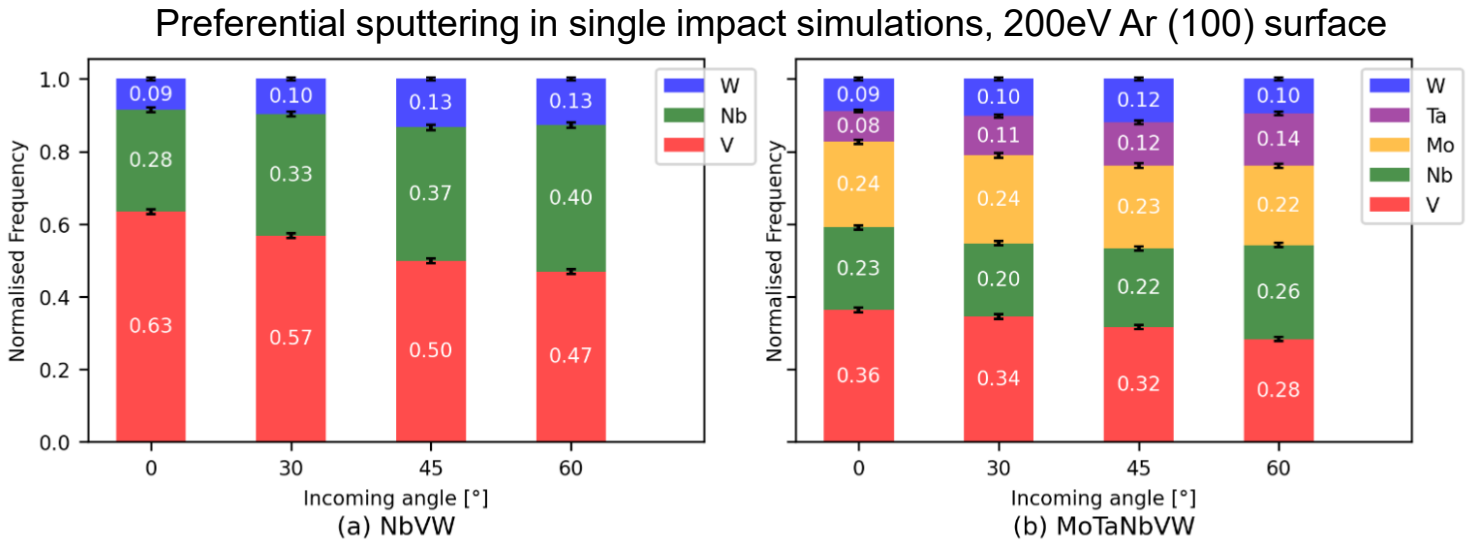


- Sputtering yields of single elemental materials quite similar
- Minimum energy for sputtering significantly more different for alloys



Sputtering of HEAs

- Preferential sputtering and surface enrichment observed
- Some increased sputtering seen for alloys compared to elemental W



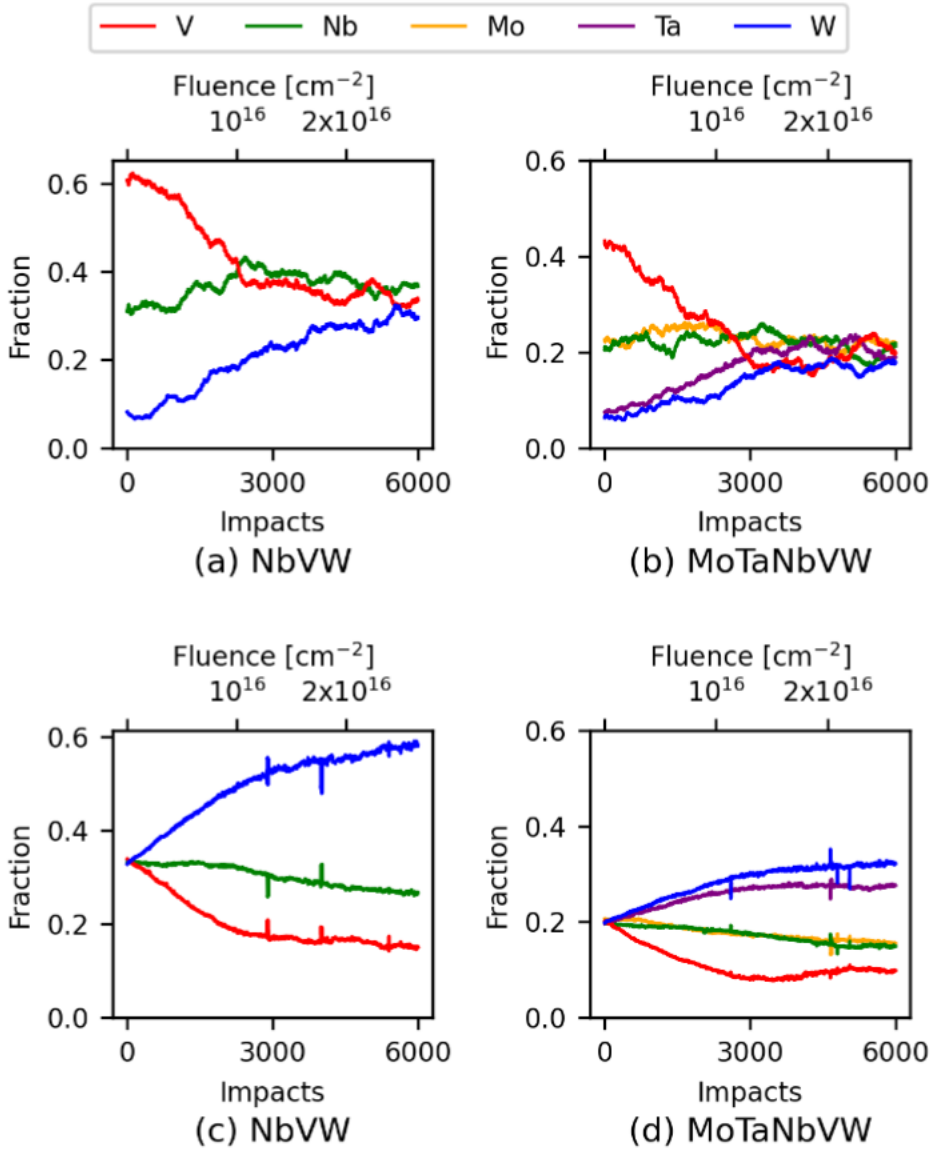


Fig. 6. Normalised preferential sputtering yield in (a) and (b), and top 15A surface composition in (c) and (d) at 200 eV and for [1 0 0] surfaces orientation over 6000 impacts

Sputtering of W-B

- Single impact results for B and W ions onto different B and W surfaces

Sputtering by 200eV perpendicular

B ion

alphaB	0,06
BetaB	0,09
WB B	0,23
W	0,006
W (100)	0,08
W (110)	0,13
W (111)	0,05
W (112)	0,07

W ion

alphaB	0,00
BetaB	0,00
WB B	0,12
W	0,002
W (100)	0,24
W (110)	0,25
W (111)	0,25
W (112)	0,26

Sputtering by 1000eV perpendicular

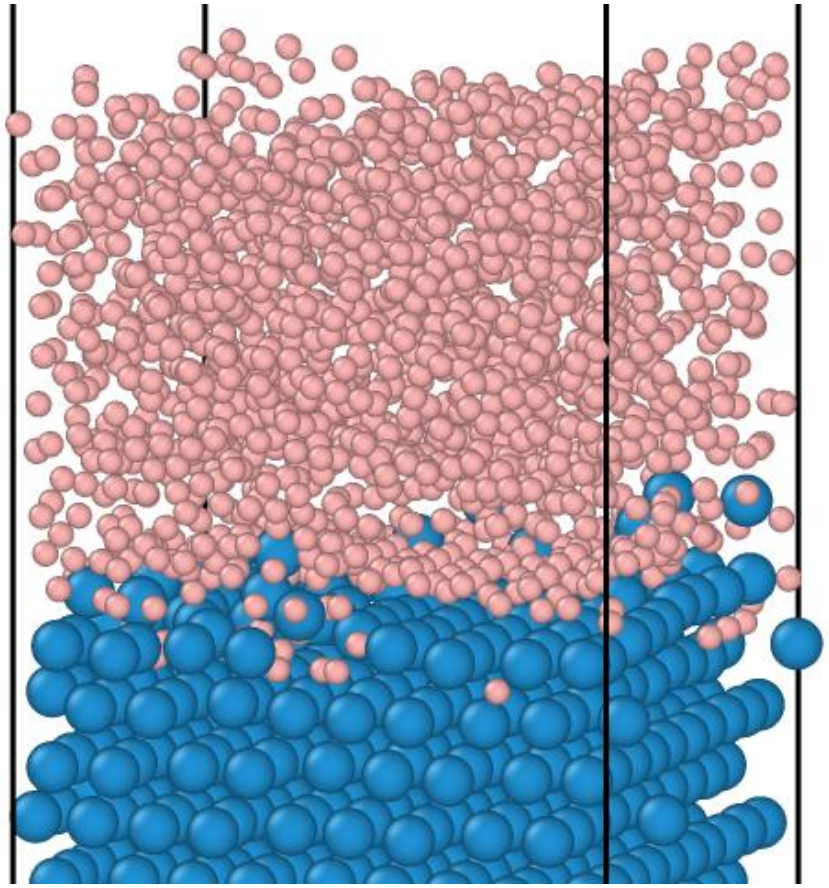
B ion

alphaB	0,24
BetaB	0,26
WB B	0,16
W	0,02
W (100)	0,17
W (110)	0,33
W (111)	0,13
W (112)	0,23

W ion

alphaB	0,16
BetaB	0,15
WB B	0,57
W	0,16
W (100)	1,52
W (110)	1,51
W (111)	1,28
W (112)	1,29

Deposition of B and sputtering of W-B



- Borophene forms during deposition
- Single vs cumulative B impacts show dramatic differences
  - Especially the WB sample

		Single		Cumulative	
500eV	alphaB		0,14		0,17
	BetaB		0,17		0,11
	WB	B	0,18		0,67
		W	0,007		0,02
1000eV	alphaB		0,24		0,25
	BetaB		0,26		0,21
	WB	B	0,16		0,61
		W	0,02		0,06

Conclusions

- We have a practically finished W-B potential
- We have a good, but not perfect, W-O-H potential
- D will weaken the W-W bonds, and therefore increase sputtering of D-decorated surfaces
- Preferential sputtering can be huge in W-B and also more complex alloys
  - Usually a saturation is observed, where surface enrichment compensate lower sputtering yield of a certain element
- Single impact simulations might not be representative, already shown before, but seen again for the W-B system especially

Current and future work

- Finalize the potentials for W-B and W-O-H, and publish them
- Carry out simulations with these
  - Boron deposition and subsequent sputtering
  - Sputtering of H and O decorated tungsten surfaces

- (2027) Combine the ML potentials to a W-B-H(-O) potential

- Within TSVV-D: Surrogate models based on MD data