MD simulations of D supersaturated W and interatomic potential development for W-O and W-O-D

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Personnel changes from proposal

- PI: Fredric Granberg (Minor or no official workload)
- Ph.D. Student: Narges Ghasemi (~6pm / year)

OUR TASK

- Excerpt from the proposal:

In order to provide ERO simulations with DEMO-relevant W erosion yields, including molecular sputtering yields, an extensive set of MD simulations will be performed for W under D/T super-saturation conditions. Existing W-H interatomic potentials that were proven to work well for PWI with W will be used for this task. Further effort will be put on development of W-O and W-O-H interatomic potentials that will be able to provide necessary input for ERO simulations under DEMO conditions when surfaces have been oxidized, e.g. as a result of off-normal transient events.

TIMELINE
Proposal

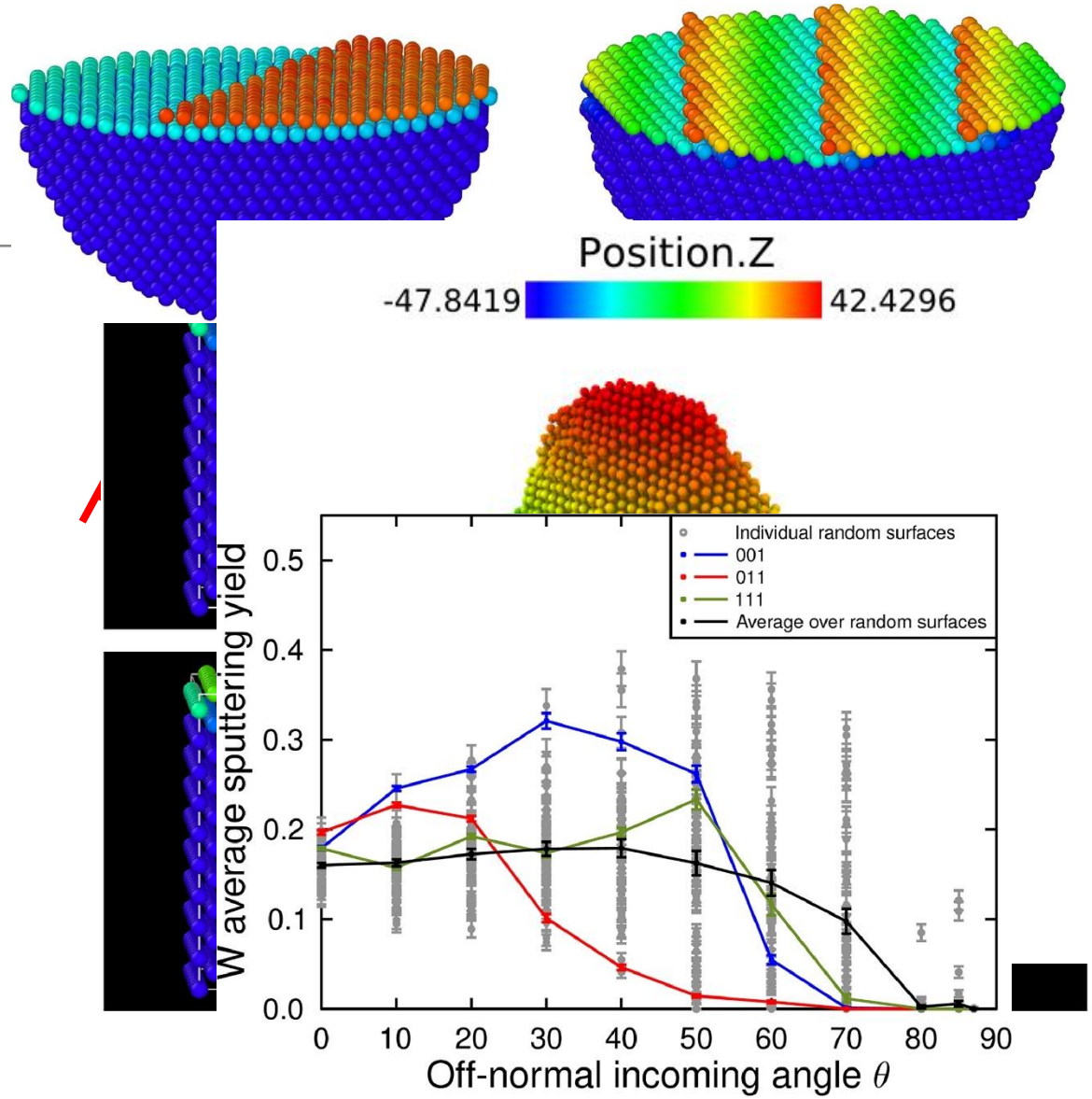
- Y1:
  - Intermediate results on erosion of H supersaturated W from MD simulations are reported
- Y2:
  - Final results on erosion of D/T supersaturated W from MD simulations are reported.
- Y3:
  - Intermediate results on W-O potential development are reported
- Y4:
  - Final results on W-O potential development are reported
  - Intermediate results on W-O-H potential development are reported
- Y5:
  - Final results on W-O-H potential development are reported

Task 1

Task 2

TASK 1
Background

- We have studied the
  - Effect of random surface orientation
  - Effect of ion element and ion energy
  - Effect of incoming angle
  - Effect of surface roughness
  - Effect of interatomic potential
  - Effect of amorphous surface
- On the
  - Sputtering and reflection yield [1,2,3,4,5]
- And identified the mechanisms



TASK 1
First steps

- Utilize existing interatomic potentials for W-H(D,T) to simulate supersaturated W surfaces under irradiation with classical Molecular Dynamics
- Develop a methodology for obtaining representative supersaturated surfaces
- Simulate single impacts from low (10-100eV) to high (1keV +) energy at different incoming angles for different surface orientations and varying supersaturation
  - Identify the mechanisms behind the sputtering phenomena
- Start cumulative impact simulations on selected similar cells as single impacts
  - Shown to yield comparable results with experiments
- Run 10,000,000 - 100,000,000 MD impacts for good statistics

TASK 2

- Expected start mid-late 2022
- Develop an interatomic potential for W-O and extend it further to W-O-H
  - At the moment very few methodologies exist for this
- Most likely a Machine Learning potential will be created
  - Previous effort for ”classical” interatomic potential generation showed to be very hard
- Drawback of ML potentials are their CPU-cost, 10-1000x slower than normal ones
  - Most interesting cases and results from TASK 1 will be validated and further investigated
  - Maybe GPU enabling will remedy the high demand and more cases can be studied
- On the side, run Task 1 like simulations with the new potential

OUR ACH REQUEST!

THANK YOU FOR YOUR ATTENTION

- References:

[1] Jussila, J., Granberg, F., and Nordlund, K. Nuclear Materials and Energy. 17 (2018) 113-122

[2] Granberg, F., Litnovsky, A., and Nordlund, K. Journal of Nuclear Materials 539 (2020) 152274

[3] Schlueter, K., Nordlund, K., Hobler, G., Balden, M., Granberg, F., Flinck, O., da Silva, T. F. and Neu, R. Physical Review Letters 125 (2020) 225502

[4] Granberg, F. and Byggmästar, J. Computational Materials Science 188 (2021) 110134

[5] Several publications in preparation