Deuterium effect on defect evolution in tungsten, from bulk to surfaces

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Acknowledgement

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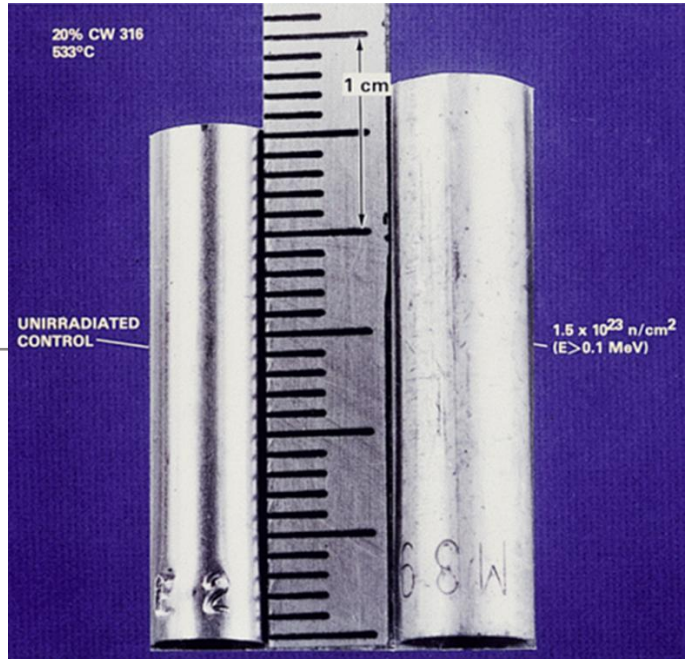
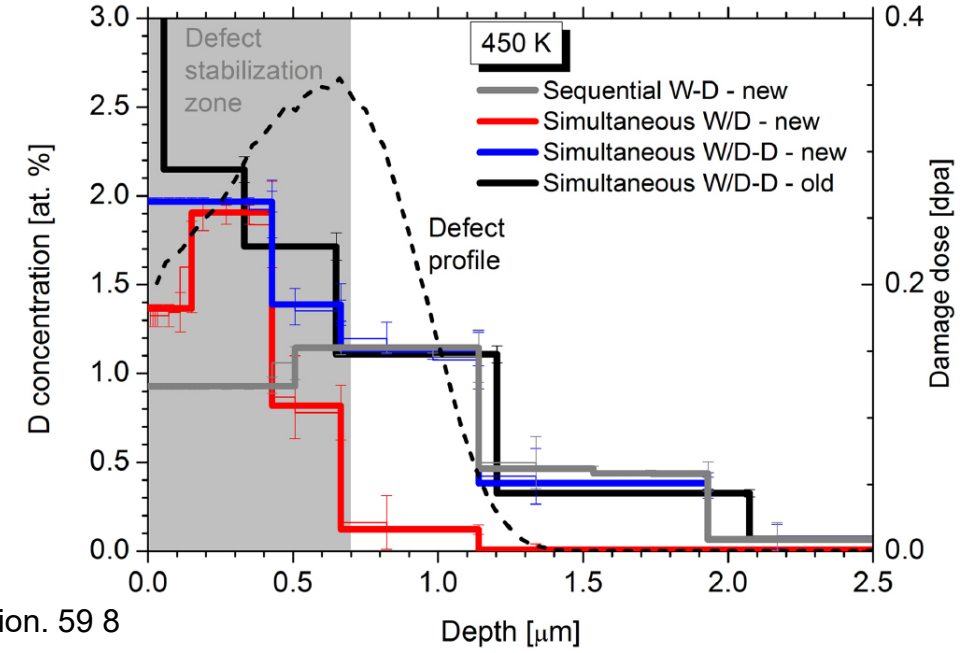
INTRODUCTION



Straalsund J L, et al. J. Nucl. Mater. 108/109 299-305 (1982)

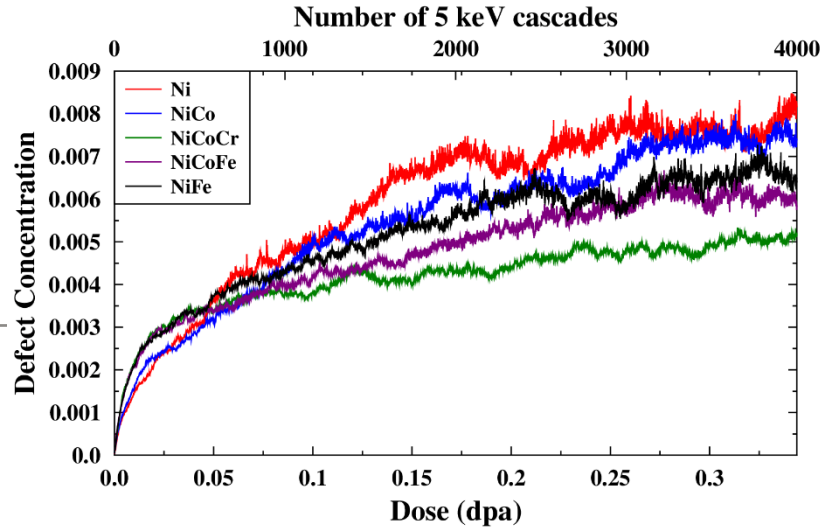
- Defects produced by irradiation do change dramatically the mechanical properties of metals
  - The defects form on nanoscale will ultimately affect macroscopic properties
  - The defects do evolve as the dose increases
- Deuterium present will affect defect build-up and retention in tungsten
  - More deuterium is retained in the sample if irradiated simultaneously with deuterium



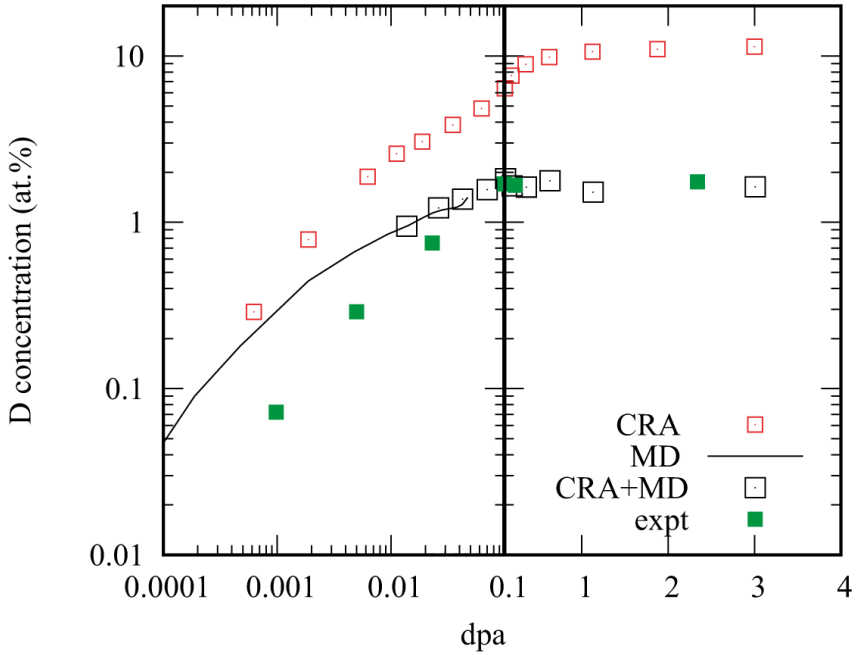
Markelj, S. et al. Nucl. Fusion. 59 8 086050 (2019)

INTRODUCTION

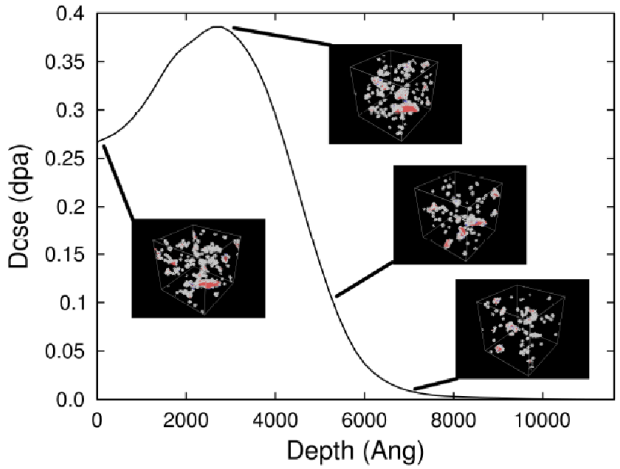
- High-dose simulations and validation

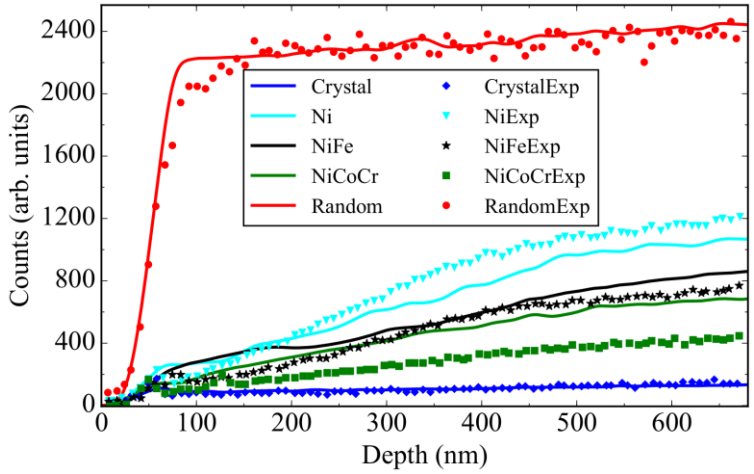


E. Levo et al. Journal of Nuclear Materials. 490 (2017) 323-332



D. R. Mason et al. Phys. Rev. Mater. 5 (2021) 095403





S. Zhang et al. Materials Research Letters. 5 (2017) 433-439

INTRODUCTION

- High energy impacts (with ML potentials)

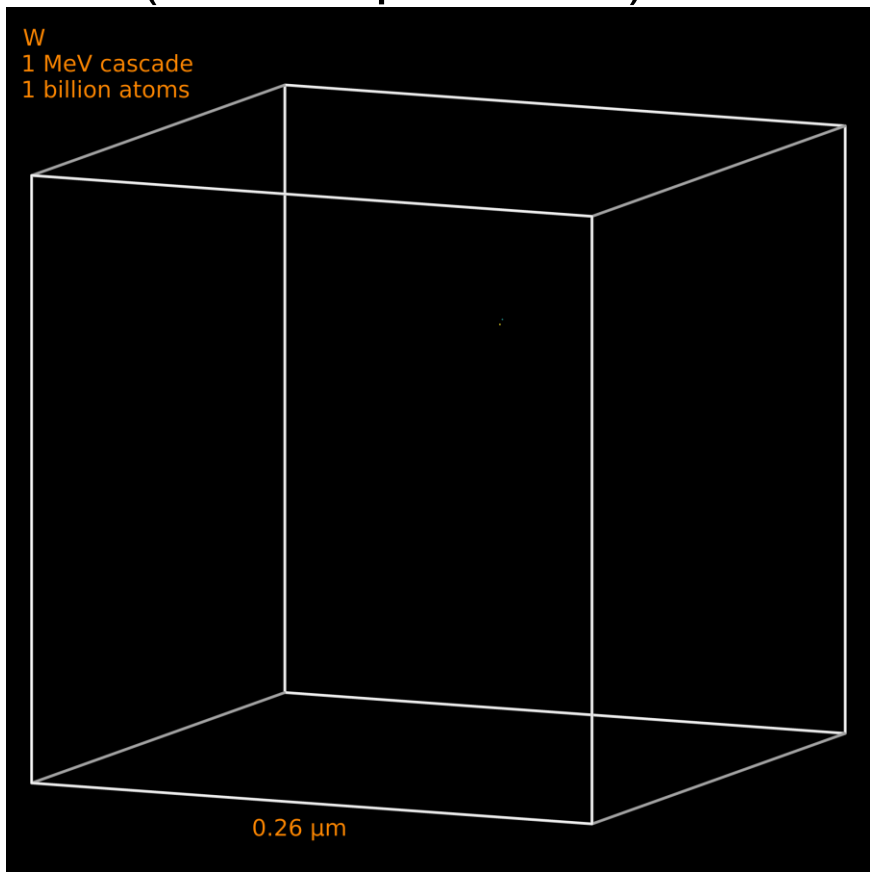
10 keV:

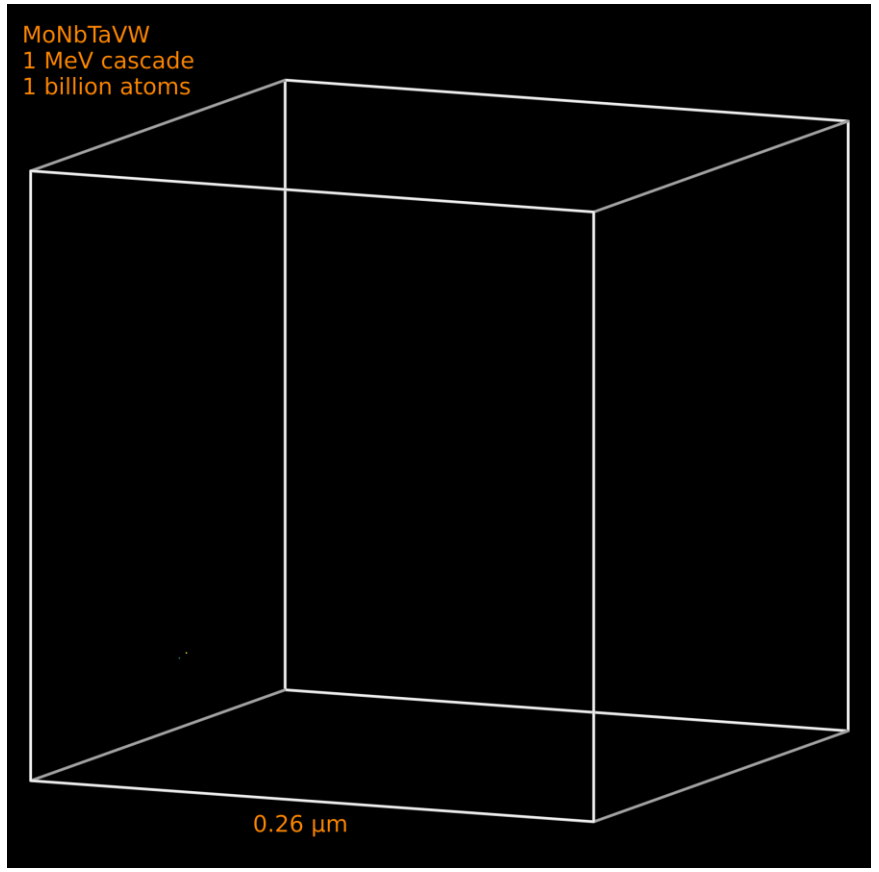
1 Million atoms

1 MeV:

1 Billion atoms

Courtesy of J. Byggmästar

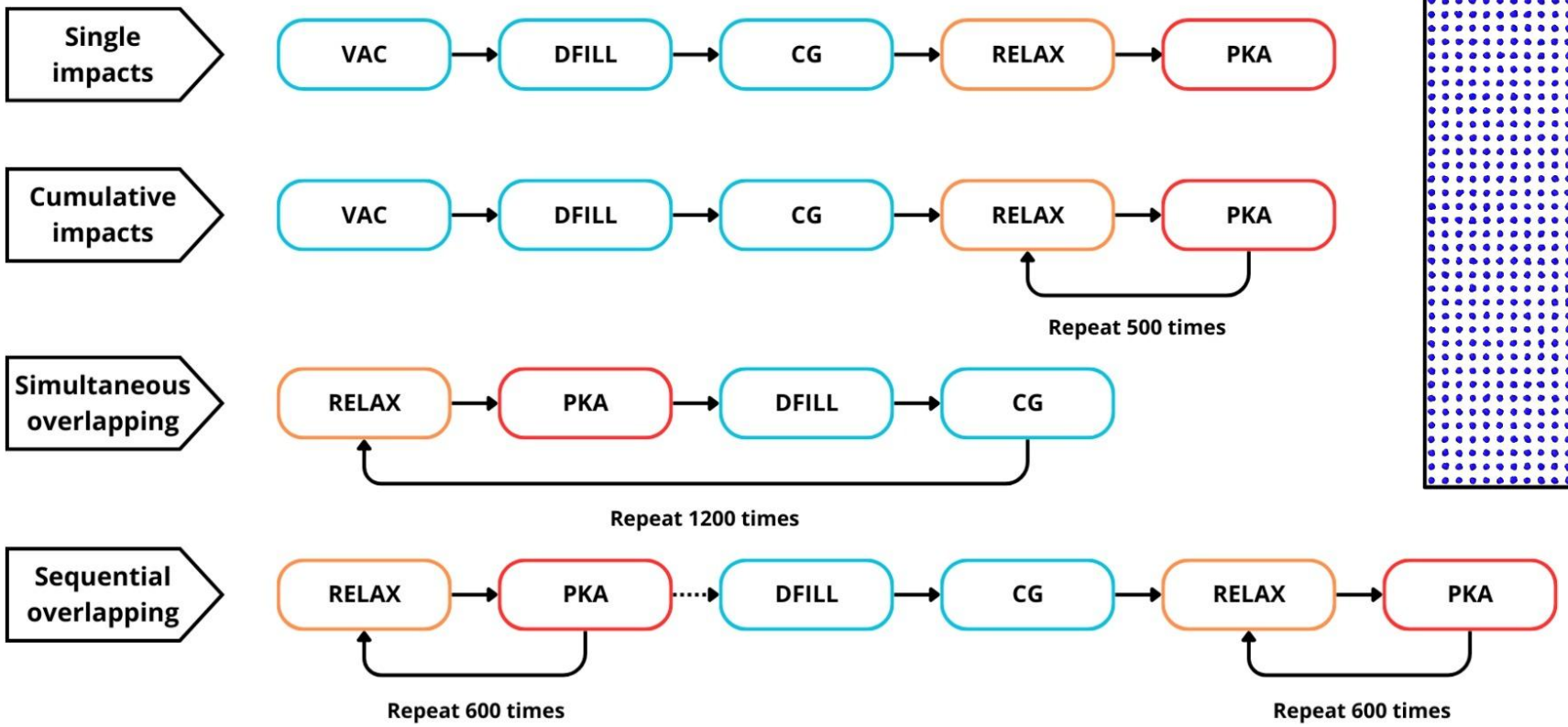


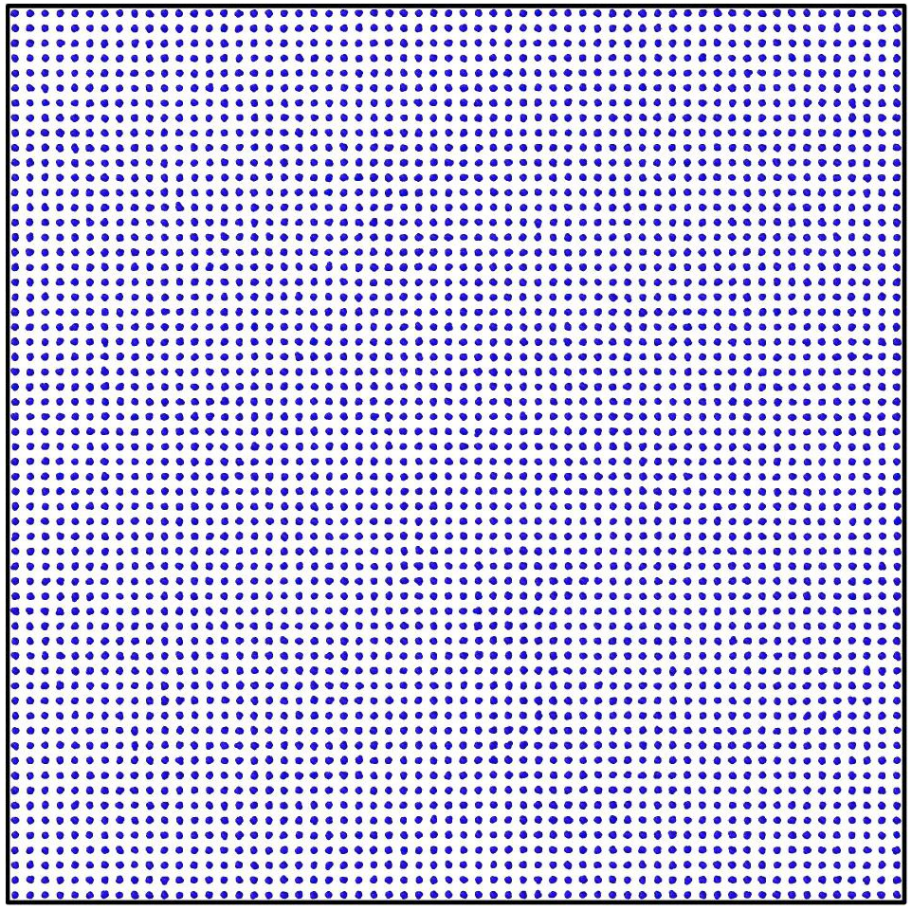


METHODS
General

- Classical MD with PARCAS and LAMMPS
- Classical potentials and ML potentials
  - Mason et al. W-H eam potential mainly in this presentation
  - Li et al. W-H tersoff-like potential also for sputtering simulations
- Single impact and massively overlapping cascade simulations
  - Various initial conditions and schemes
- In sputtering simulations, the universal repulsive ZBL-potential was used
  - For the ions argon and neon

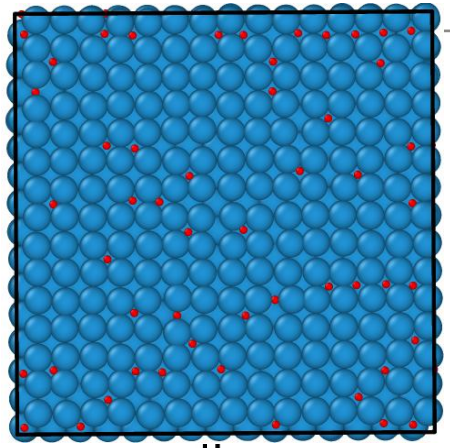
METHODS
Bulk simulations

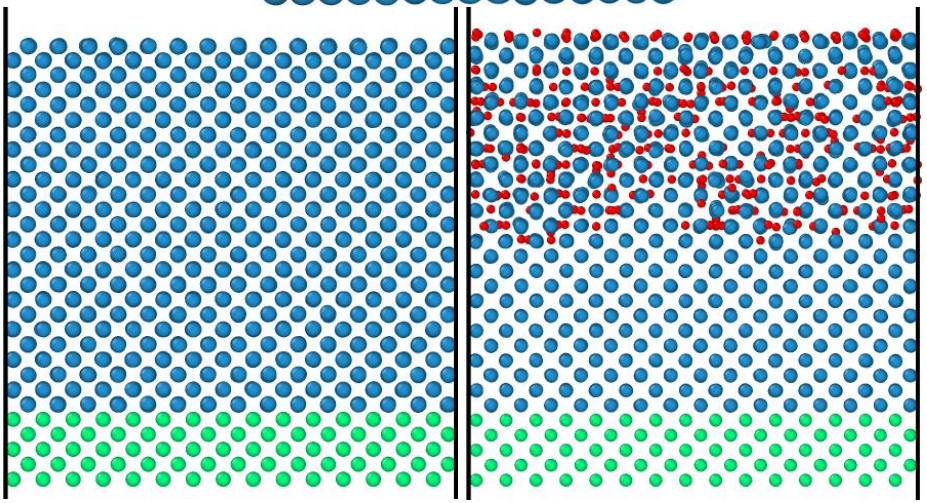




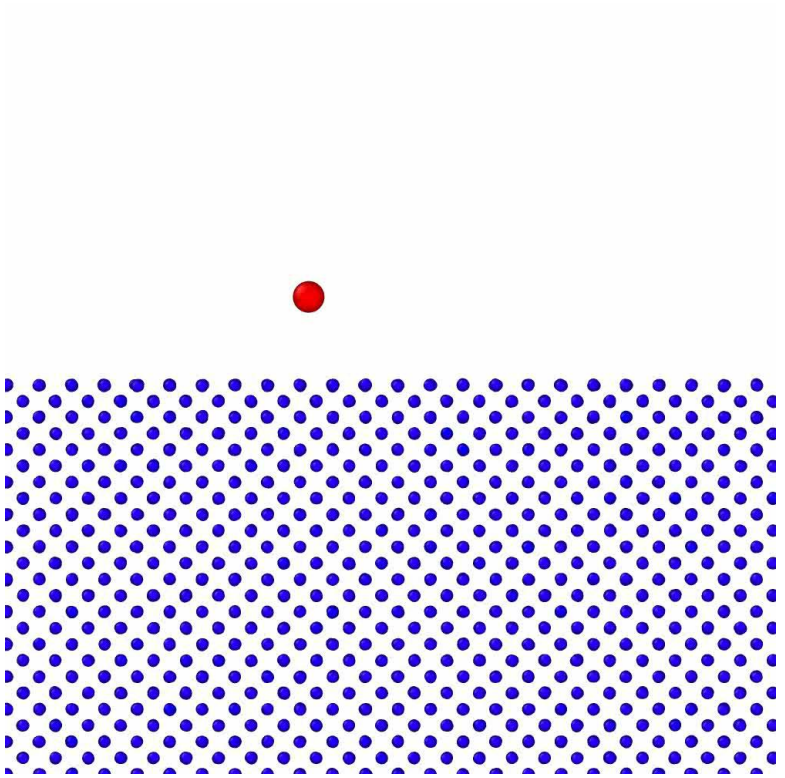
V. Lindblad et al. J. Nucl. Mater. 603 (2025) 155422

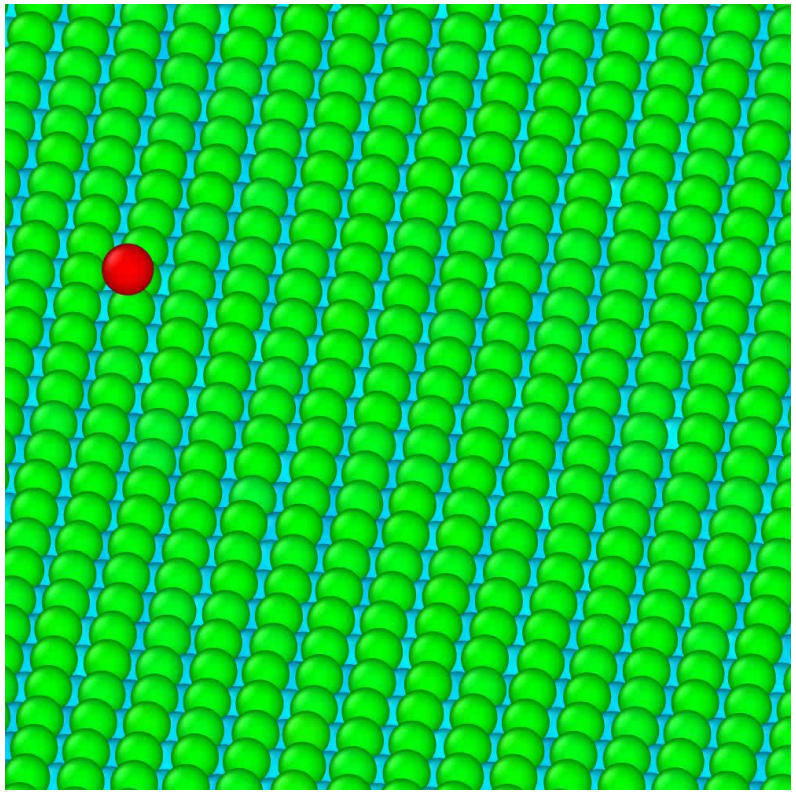
METHODS
Sputtering simulations





NOTE: Non-linear timescale

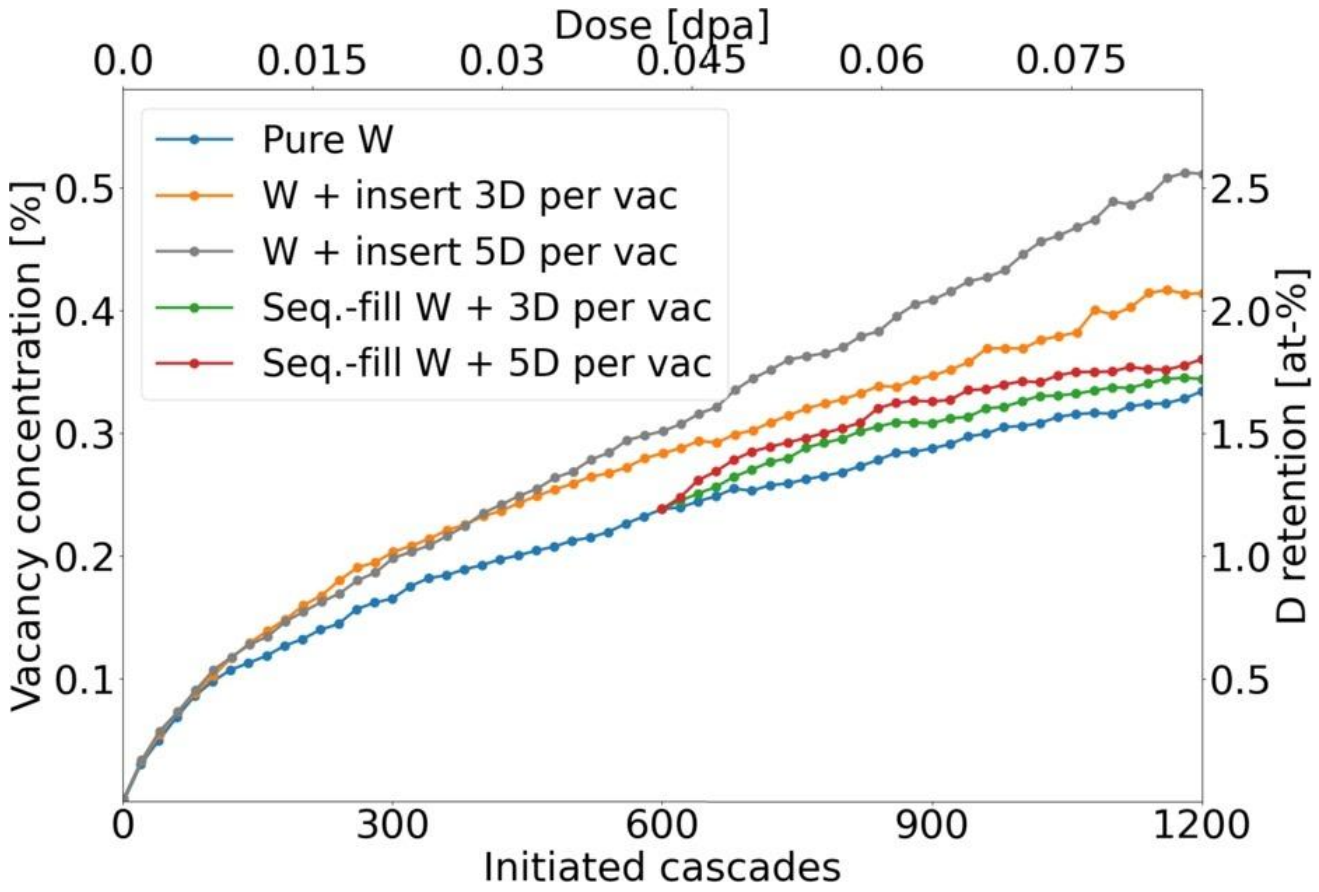




F. Kporha et al. in preparation (2025)

RESULTS
Deuterium effect on defect production

- Pure W shows least defects
- Adding deuterium in the middle temporarily increase the defect concentration
- Having all vacancies filled will dramatically increase defect concentration
- Different D-concentrations affect the magnitude



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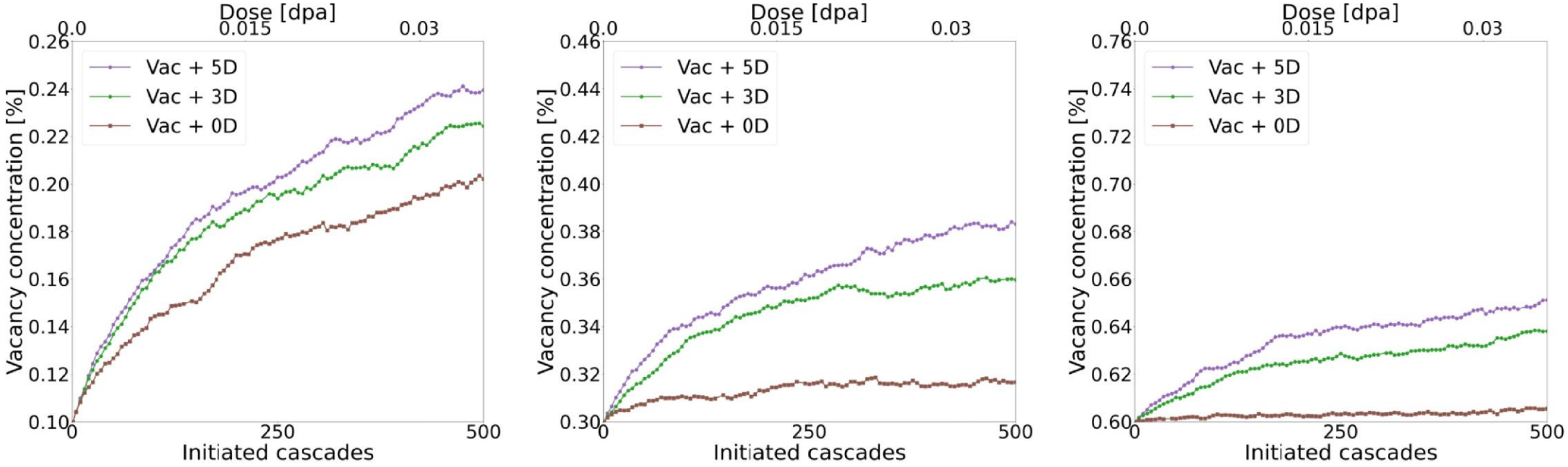
RESULTS
Deuterium effect on defect production

- We see that having vacancies affect the defect production, and the effect of deuterium in them.



(a) 0.1% initial vacancy concentration **(b)** 0.3% initial vacancy concentration **(c)** 0.6% initial vacancy concentration

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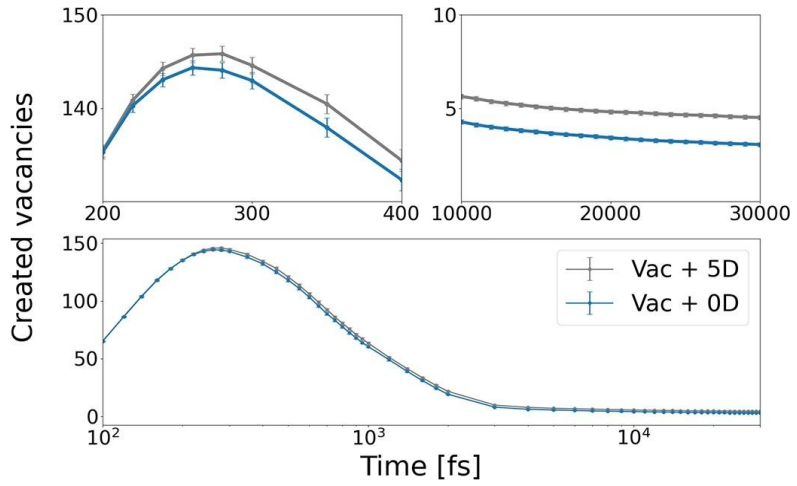
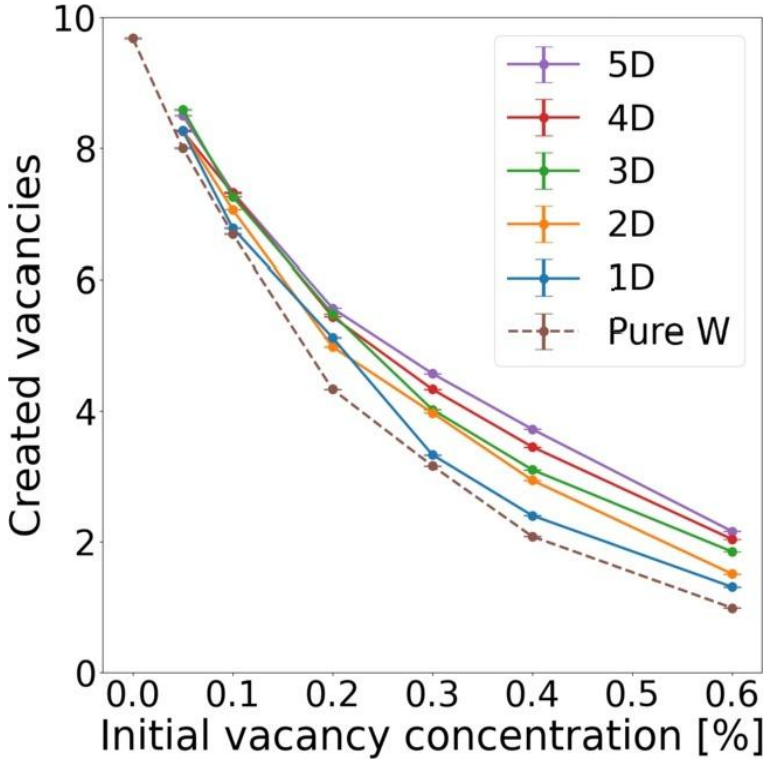
RESULTS
Deuterium effect on defect production

- Adding vacancies will decrease the number of newly created vacancies
- Filling them will reduce the effect
  - The more D, the lesser the effect
- Deuterium present also increase the number of vacancies at peak damage





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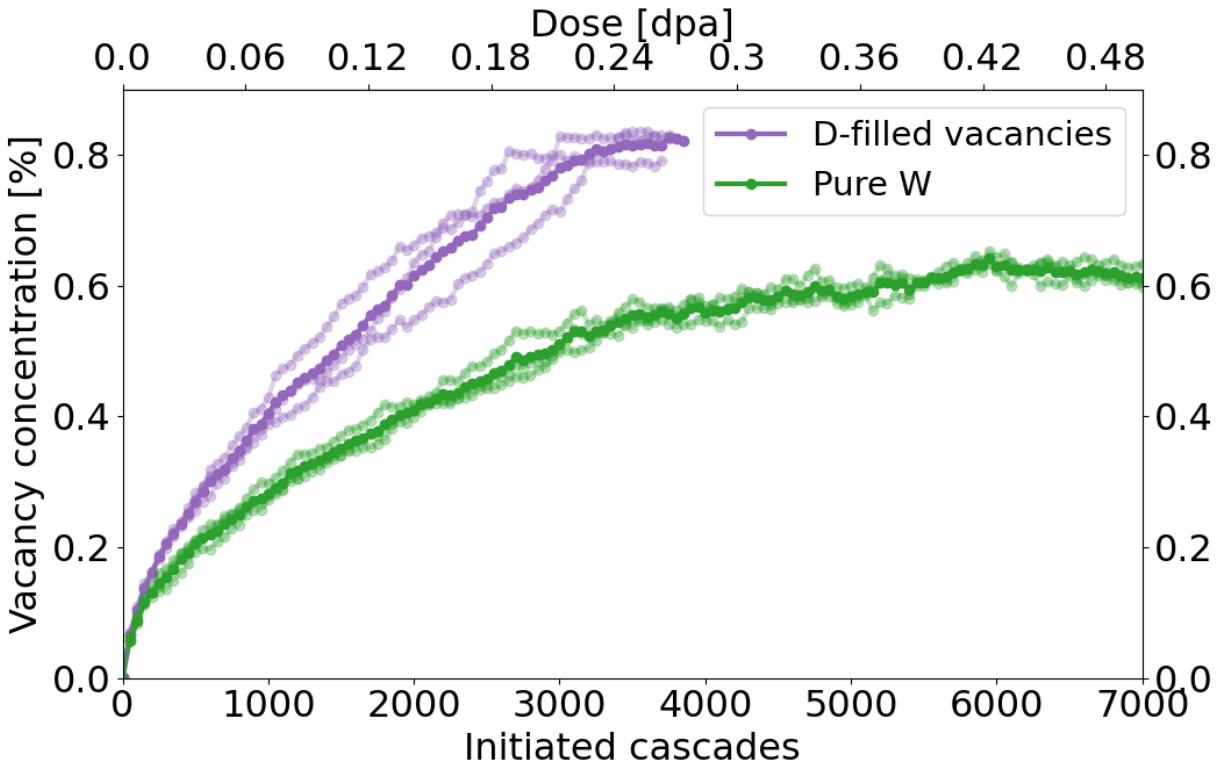
RESULTS
Deuterium effect on defect production

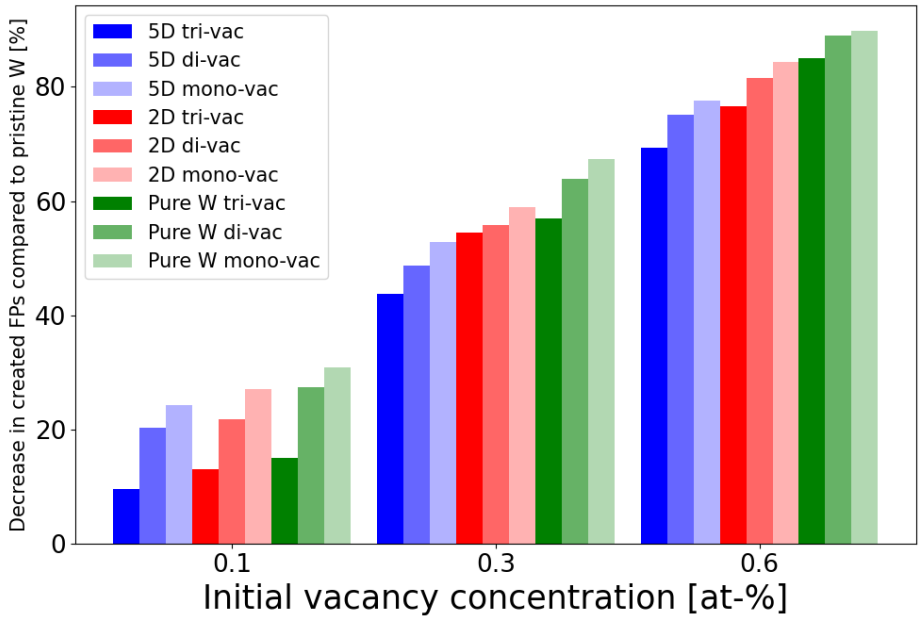
- Going to even higher dose, eg. saturation, we see a difference in vacancy concentration, where deuterium show a 30% higher saturation level

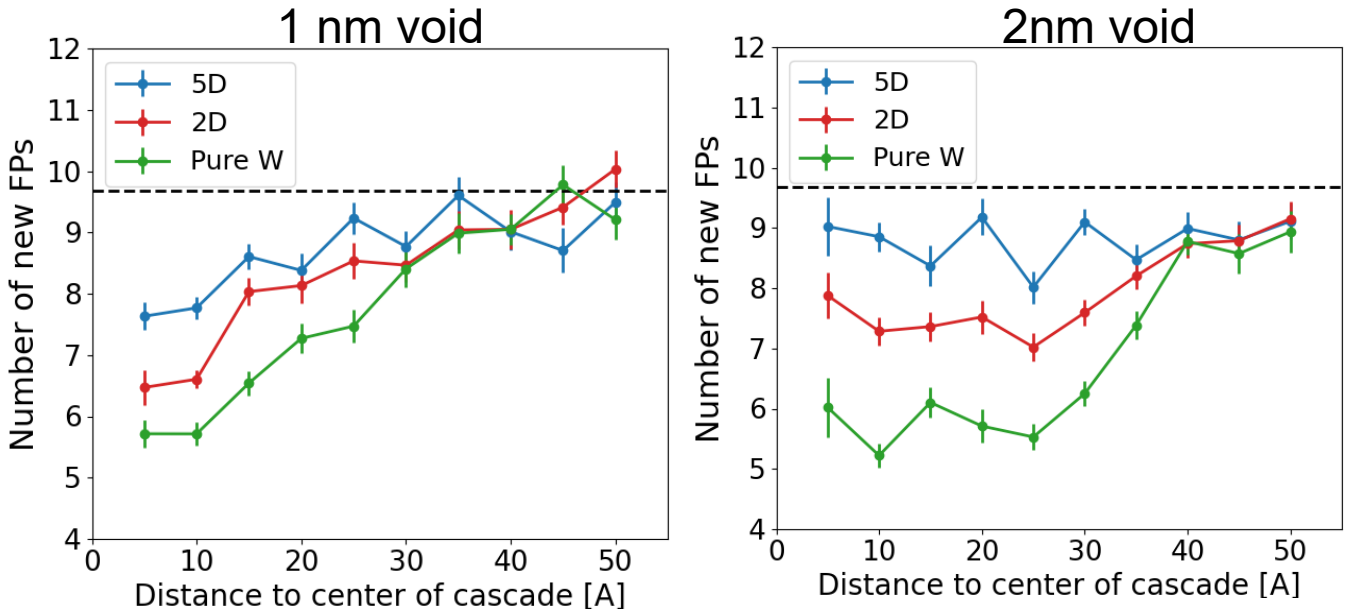


V. Lindblad & F. Granberg in preparation (2025)

RESULTS
Deuterium effect on defect production

- We see that single vacancies at a certain concentration is most effective, but di- and tri vacanices have an effect, also and effect of D-filling level
- Large voids show similar effect, but to a lesser extent



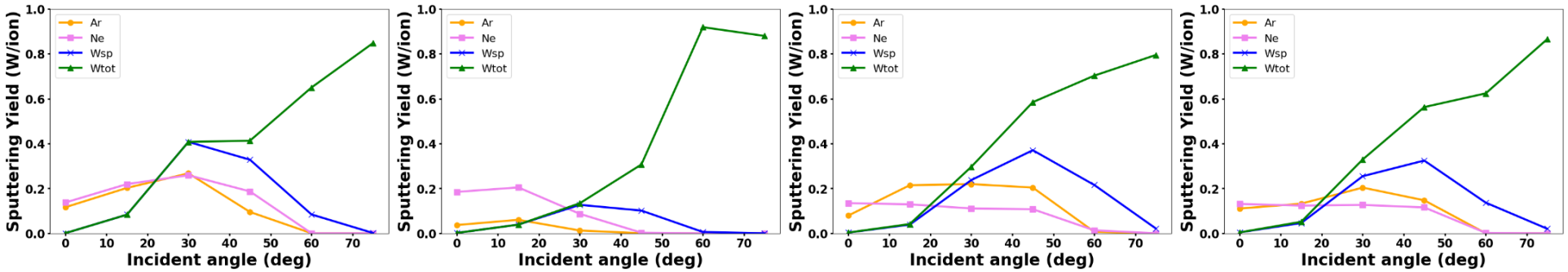


V. Lindblad & F. Granberg in preparation (2025)

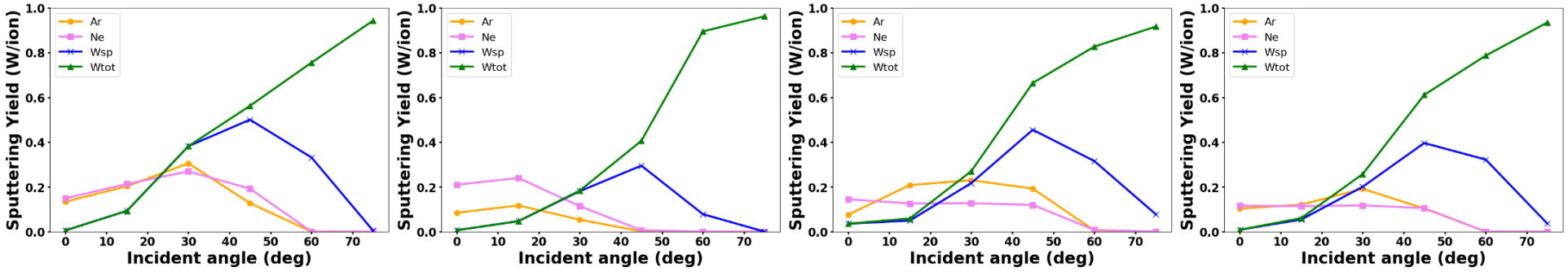
RESULTS
Pure W sputtering

- Sputtering of pristine W by different ions for different surface orientations

Mason et al.



Li et al.

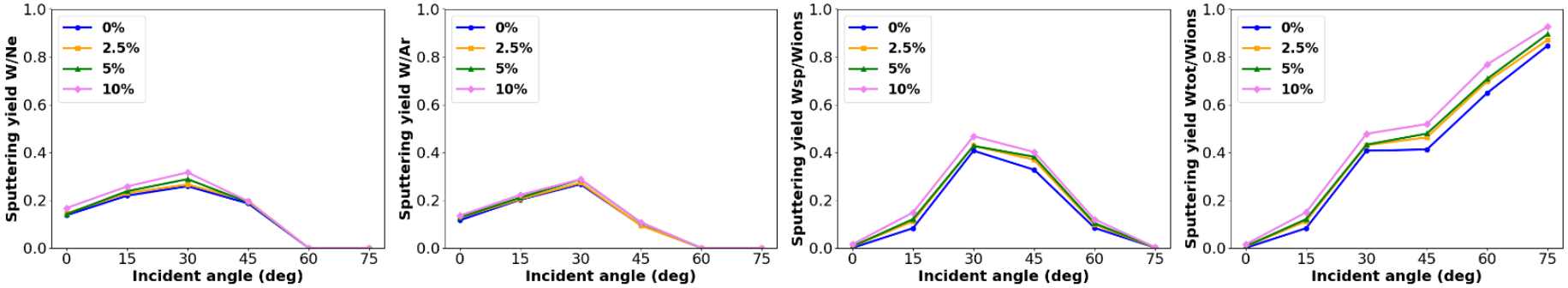


F. Kporha et al. J. Nucl. Mater. 613 155856 (2025)

RESULTS
D decoration W sputtering

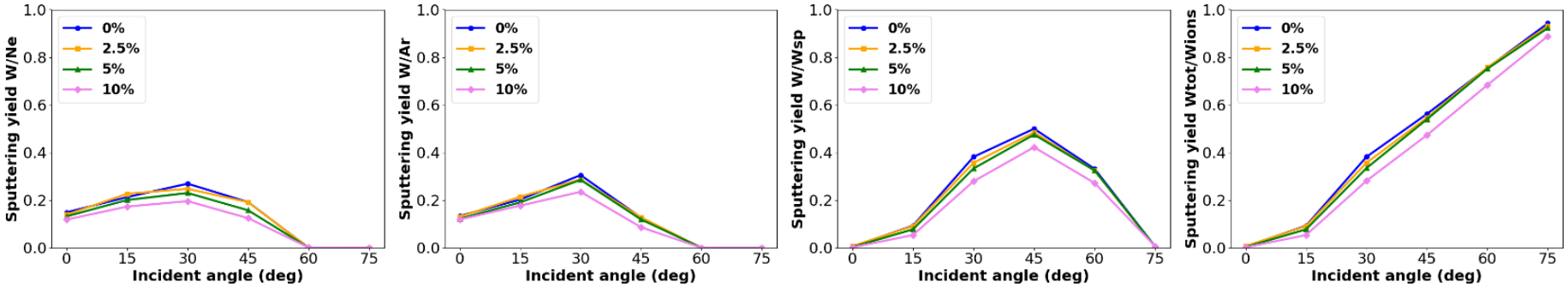
- Sputtering of (100) W by different ions for different deuterium decoration levels

Mason et al.



(a) Ne (b) Ar (c) W_{sp} (d) W_{tot}

Li et al.



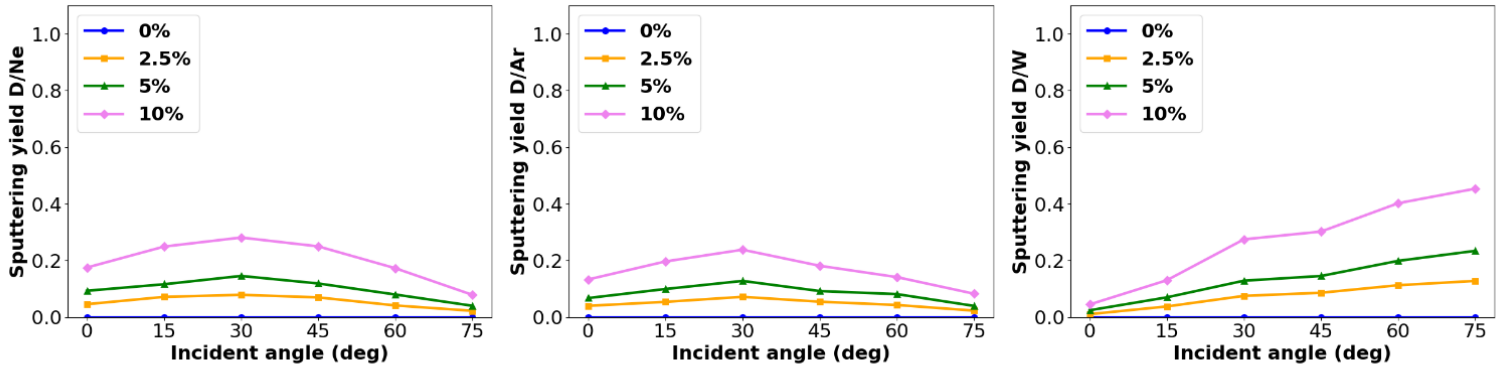
(e) Ne (f) Ar (g) W_{sp} (h) W_{tot}

F. Kporha et al. in preparation (2025)

RESULTS
D sputtering

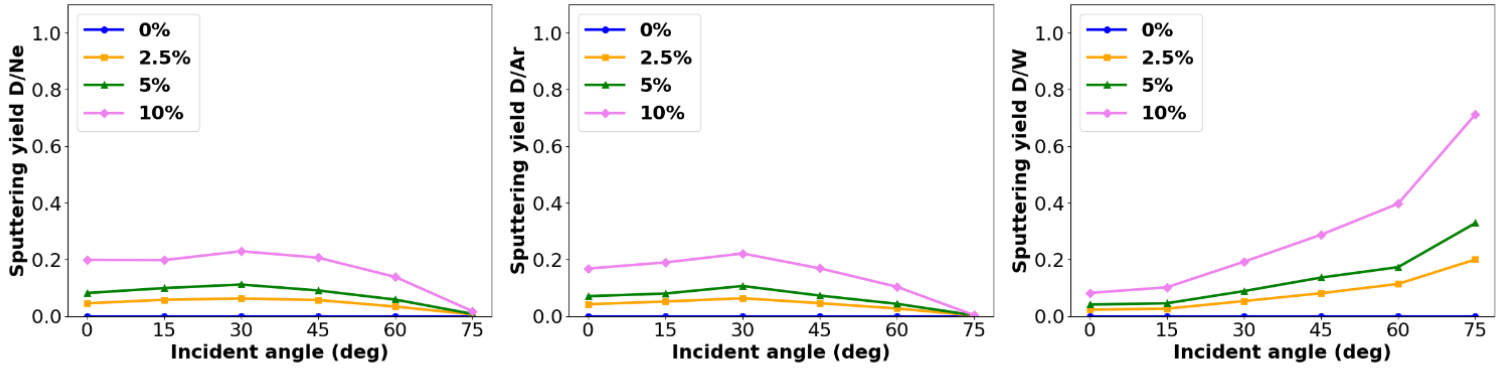
- Deuterium can sputter under most conditions, even though tungsten sputtering is practically zero

Mason et al.



(a) Ne (b) Ar (c) W

Li et al.



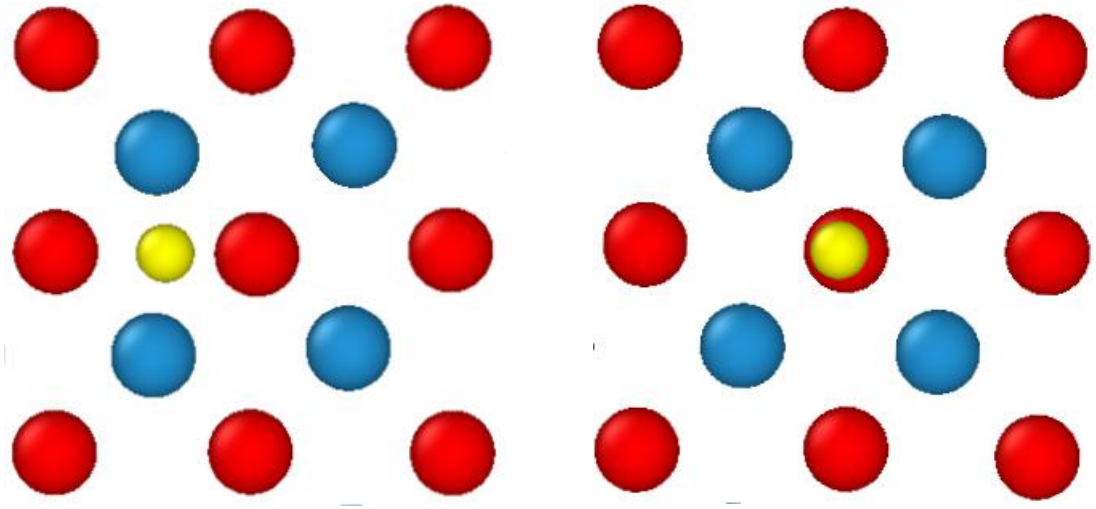
(d) Ne (e) Ar (f) W

F. Kporha et al. in preparation (2025)

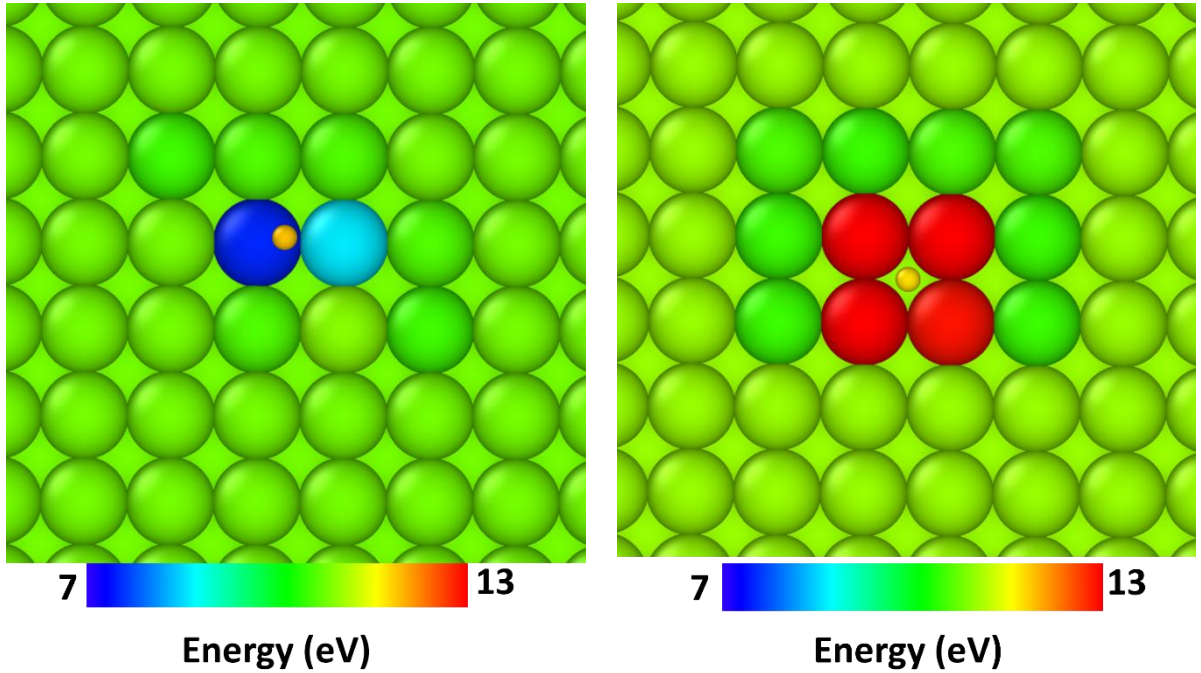
RESULTS

- Stable D position on W surfaces (100)
- Energy required for sputtering

Mason et al. Li et al.



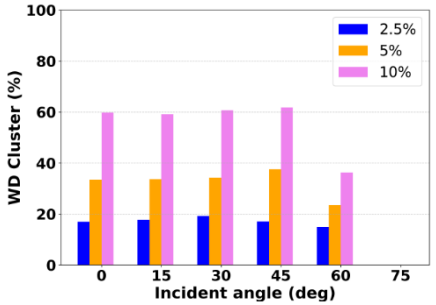
Mason et al. Li et al



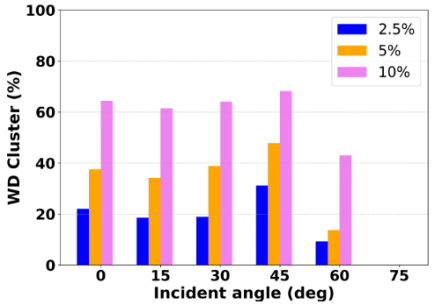
F. Kporha et al. in preparation (2025)

RESULTS

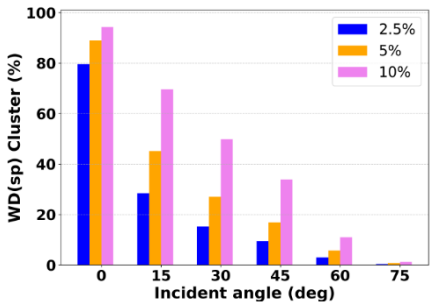
- WD cluster sputtering for various ions, angles and energies



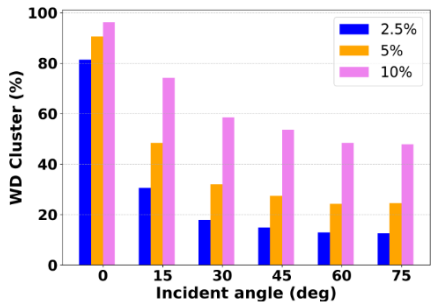
(a) Ne - 100 eV



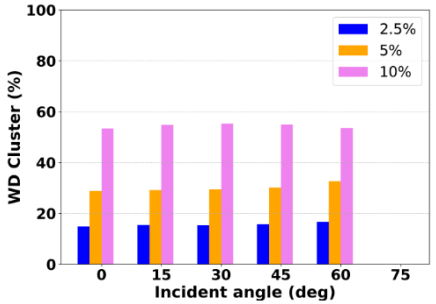
(b) Ar - 100 eV



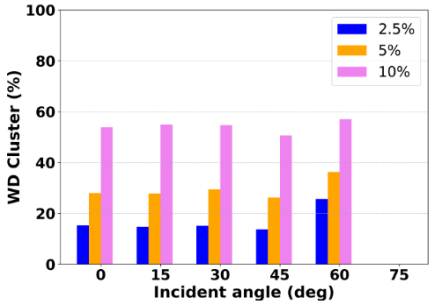
(c) W_{sp} - 100 eV



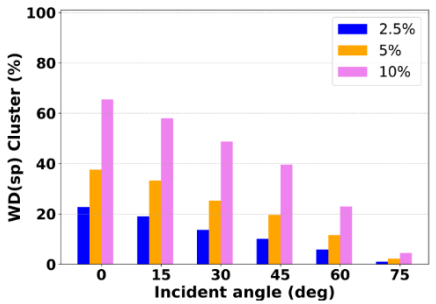
(d) W_{tot} - 100 eV



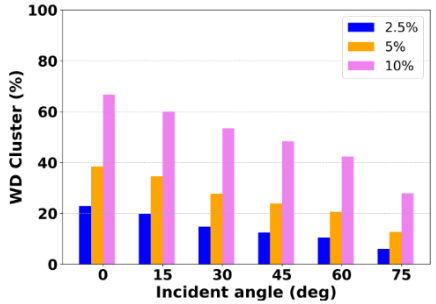
(e) Ne - 200 eV



(f) Ar - 200 eV



(g) W_{sp} - 200 eV



(h) W_{tot} - 200 eV

F. Kporha et al. in preparation (2025)

OUTLOOK
Discrepancy in classical potentials

- Classical potentials show widely different trends (for surfaces)
- We need a fast and accurate potential for surface effects

➔Tabulated Gaussian Approximation Potential (tabGAP)

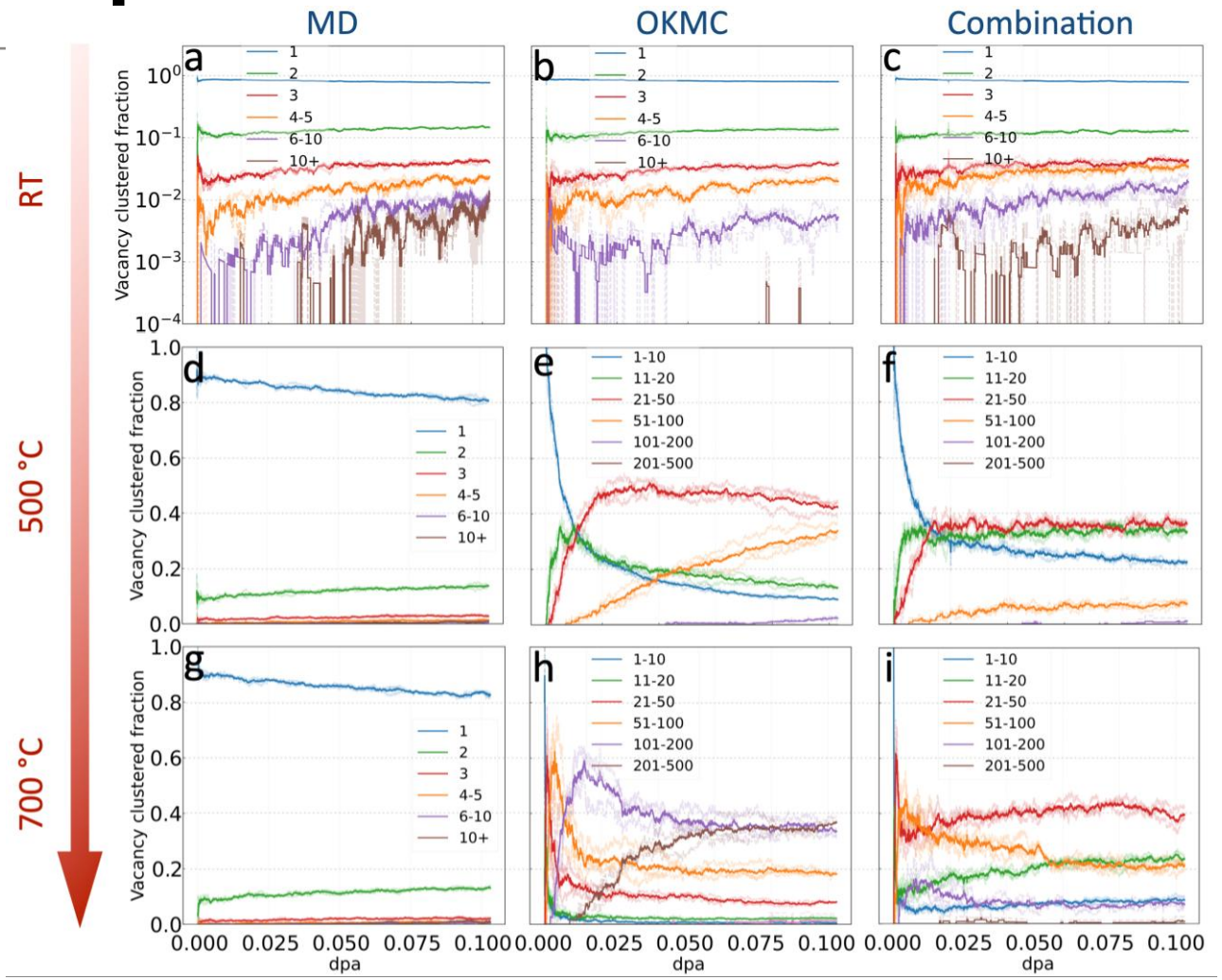
- Pure W potential exists, e.g. training data available [1]

- We are currently adding H and O, to get a W-O-H potential for sputtering simulations

[1] J. Byggmästar et al. Phys. Rev. B. 100 14 (2019) 144105

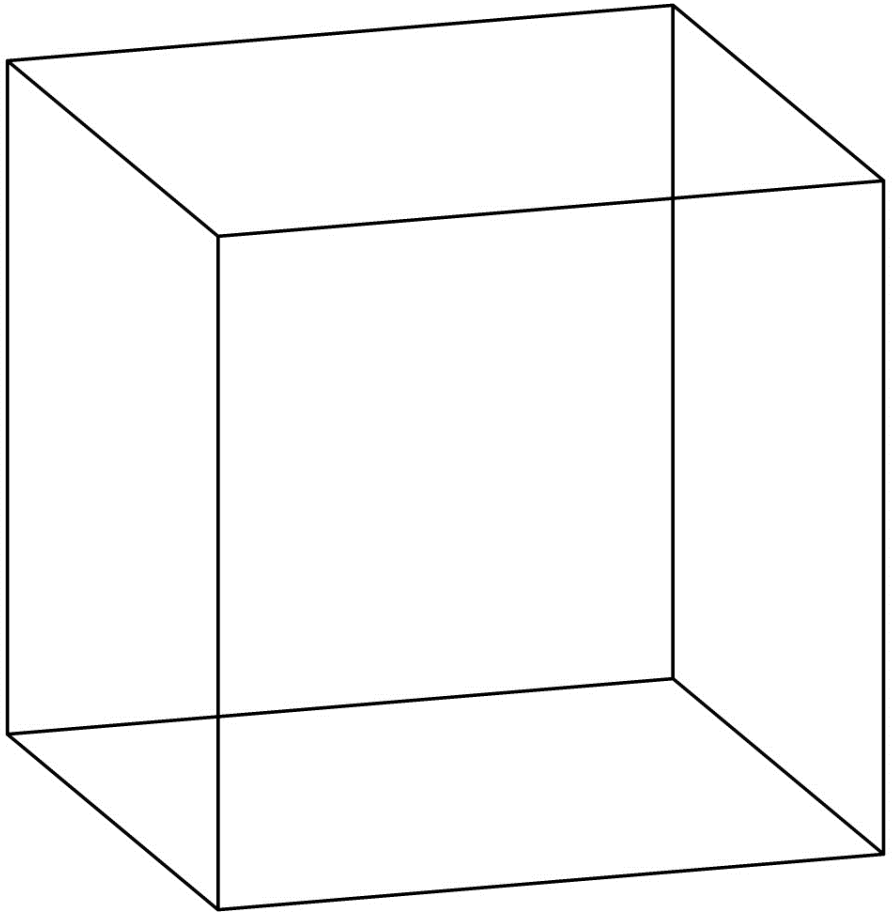
OUTLOOK
Timescale/Dose-rate problems

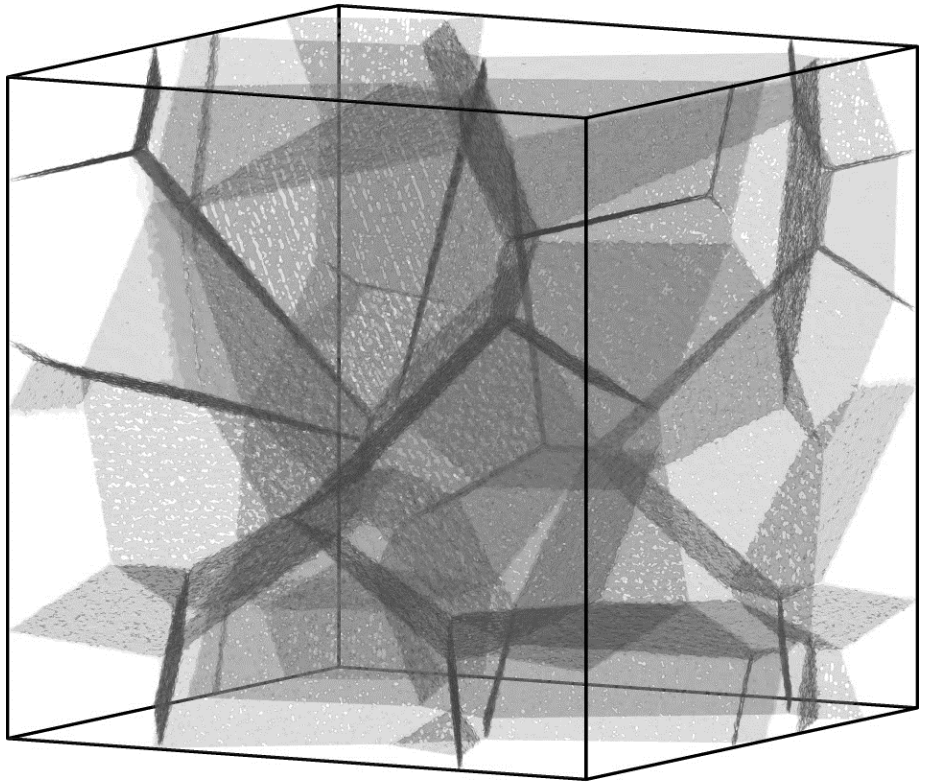
- At room temperature practically no difference between the different methods, except less clustering in pure OKMC
- At higher temperatures, when vacancies are mobile, the effect is huge
- We have a workflow for pure W, and will extend the (OKMC) database with deuterium effects



J. Wu et al. in preparation (2025)

OUTLOOK
Size does matter





CONCLUSIONS

- We have identified the mechanisms for higher defect retention in samples irradiated simultaneously by ions and deuterium
  - In line with experiments
  - Main factors are increase defect production and lesser recombination
- Sputtering simulations have revealed the deuterium on the surface will affect the sputtering of tungsten
  - Additionally, deuterium can easily sputter away from the surface

THANK YOU FOR YOUR ATTENTION

Parameter-free quantitative simulation of high dose microstructure and hydrogen retention in ion-irradiated tungsten

Mason, D. R., Granberg, F., Boleininger, M., Schwarz-Selinger, T., Nordlund, K., and Dudarev, S. L.

Physical Review Materials 5 (2021) 095403

The effect of deuterium on defect production in irradiated tungsten

Lindblad, V., Mason, D. R., and Granberg, F.

Journal of Nuclear Materials 603 (2025) 155422

Sputtering of tungsten surfaces by different ion types: a molecular dynamics study

Kporha, F., Nordlund, K., and Granberg, F.

Journal of Nuclear Materials 613 (2025) 155856

Sputtering of deuterium decorated tungsten surfaces by argon, neon and tungsten ions

Kporha, F., Byggmästar, J., Nordlund, K., and Granberg, F.

In preparation (2025)

Effect of deuterium in vacancy type defects on defect production in tungsten under irradiation

Lindblad, V., and Granberg, F.

In preparation (2025)

High-dose long-time defect evolution in tungsten studied by atomistically informed Object Kinetic Monte Carlo simulations

Wu, J., Balbuena, J.-P., Hu, Z., Jantunen, V., Barthe, M.-F., Caturla, M. J., and Granberg, F.

In preparation (2025)