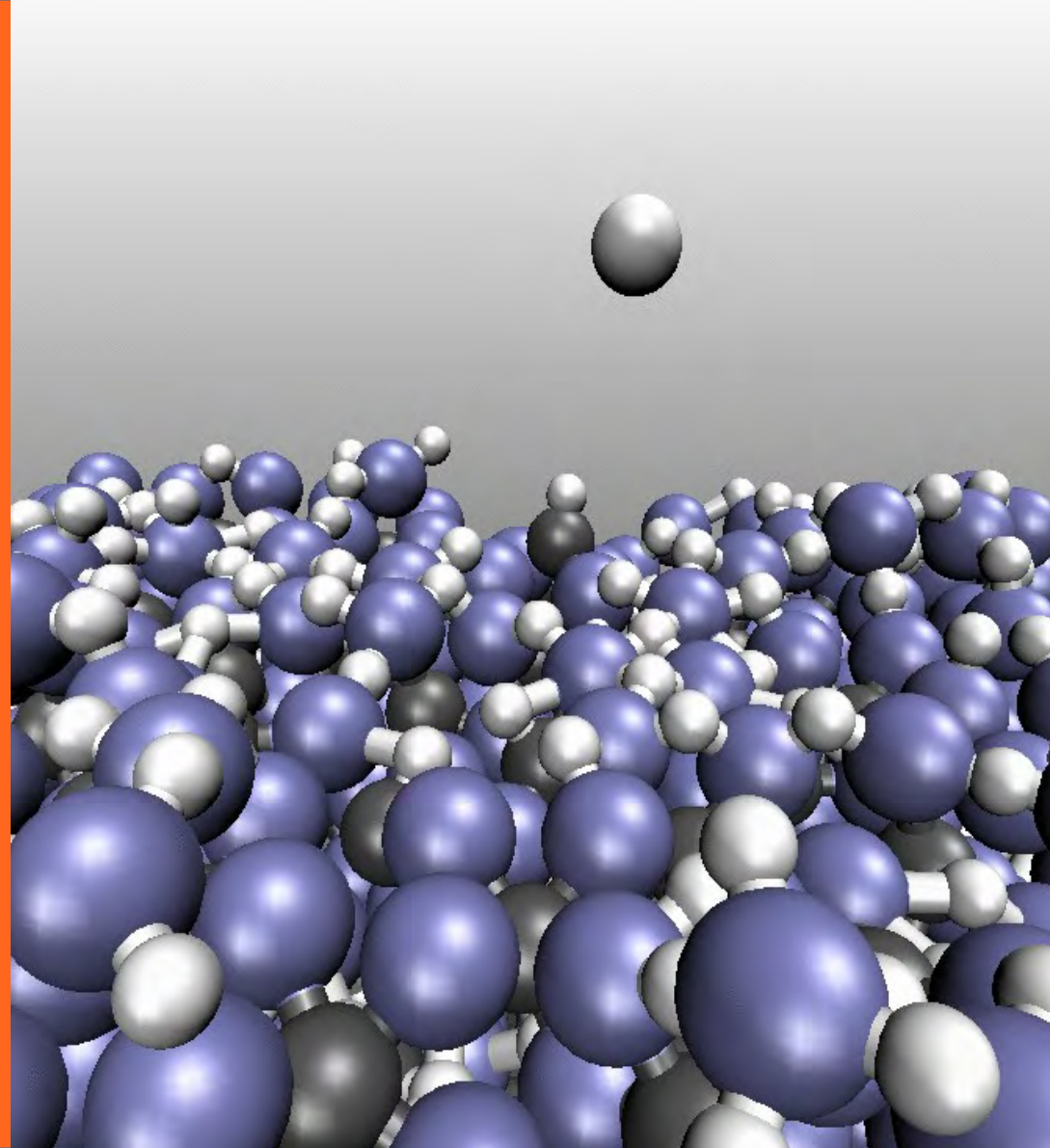


Fusion materials modelling at Aalto

Andrea E Sand
Aalto University

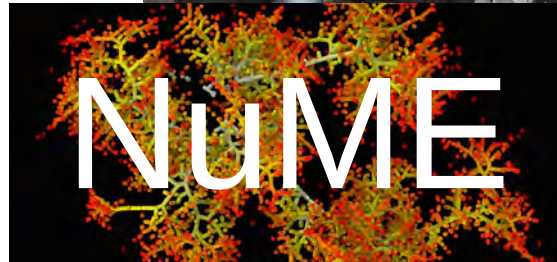


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Our team

- The Nuclear Materials and Engineering (NuME) group was established at Aalto University, School of Science Department of Applied Physics in 2021
- Computational materials physics research, focus on radiation induced processes and damage formation in materials
- Current fusion-related activities include
 - Electronic energy losses of light ions and sputtering of Fe/W (Evgeniia Ponomareva's presentation yesterday)
 - Neutron damage in tungsten under external loading conditions
 - Plasma-wall interactions for various ions/materials



Outline

- Cascade damage in tungsten under external loading conditions
- Sputtering from Be-H/D/T surfaces
- Low energy nitrogen reflection from W-N surface

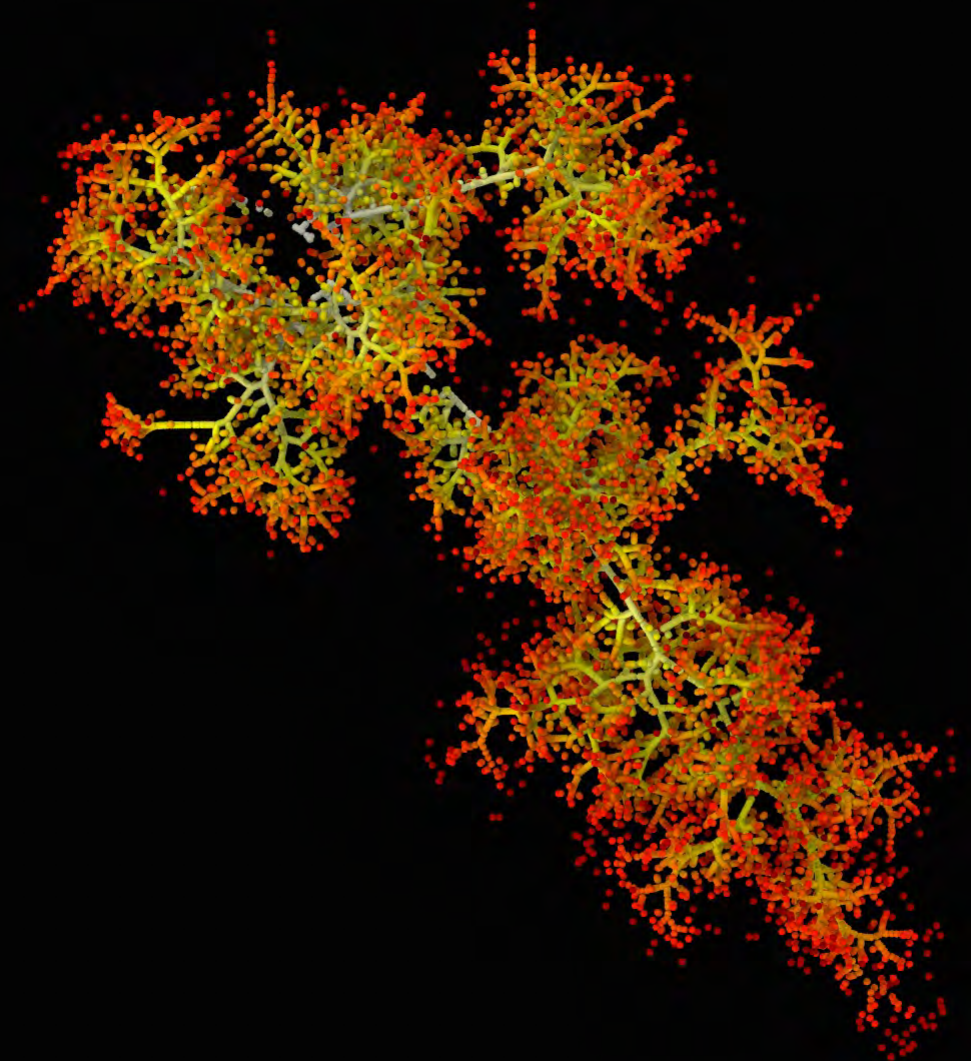
Cascade damage in tungsten under external loading



Antoine Clement, Ilja Stanovohh, Iisa Saunamäki

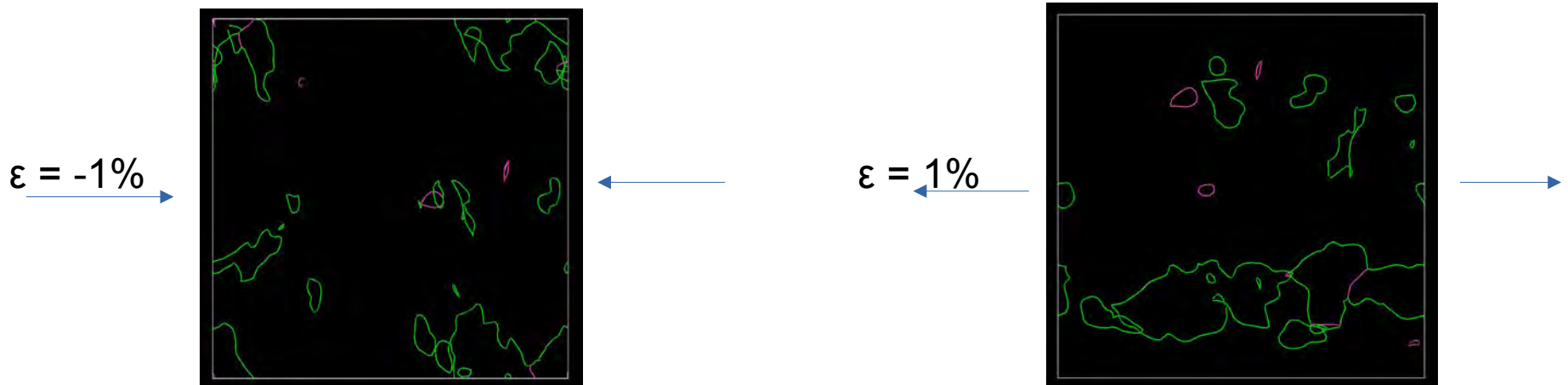


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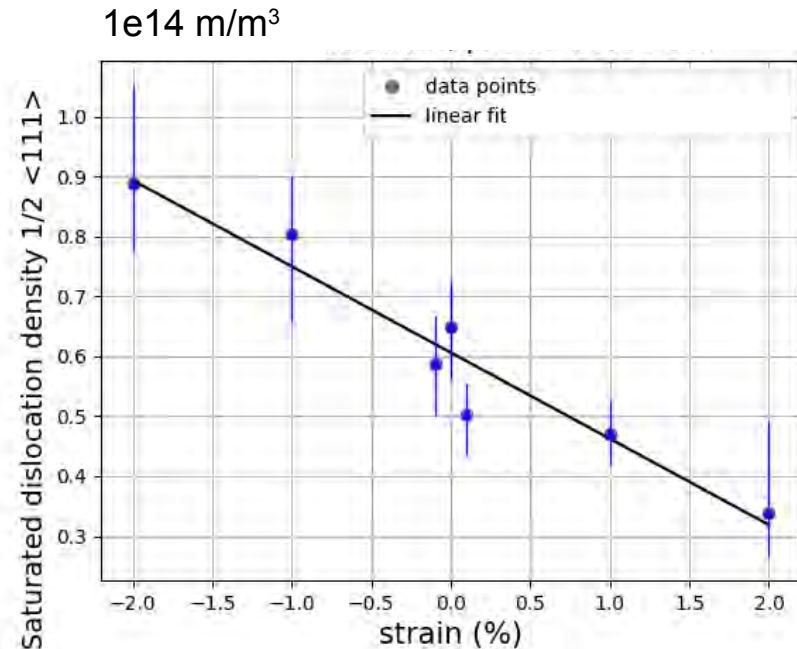
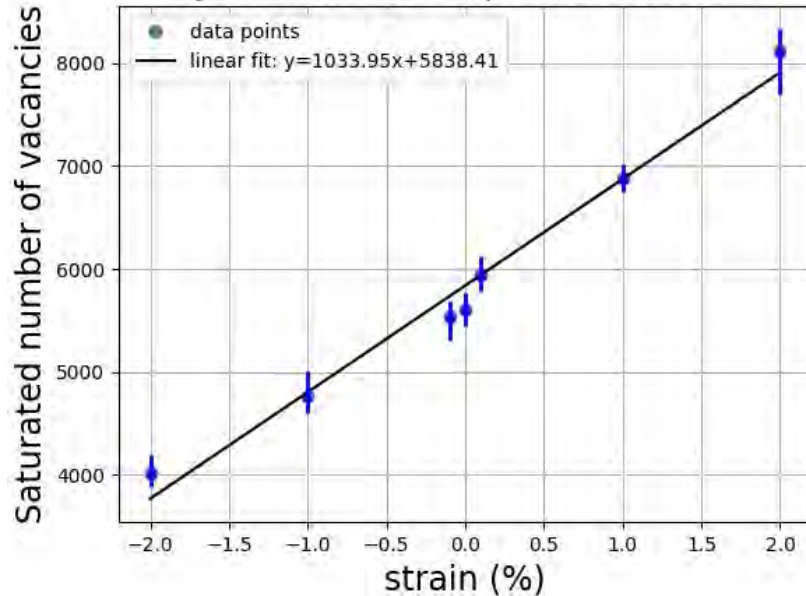
Cascades under external loading

- Cubic cells with 2M atoms
- Model of high dose microstructure constructed using Frenkel pair insertion, followed by 1500 random 10 keV cascades
- Applied strain in $\langle 100 \rangle$ direction (-2%, -1%, -0.1%, 0.1%, 1%, 2%)
- Strained system equilibrated in NVT (300K) before cascades



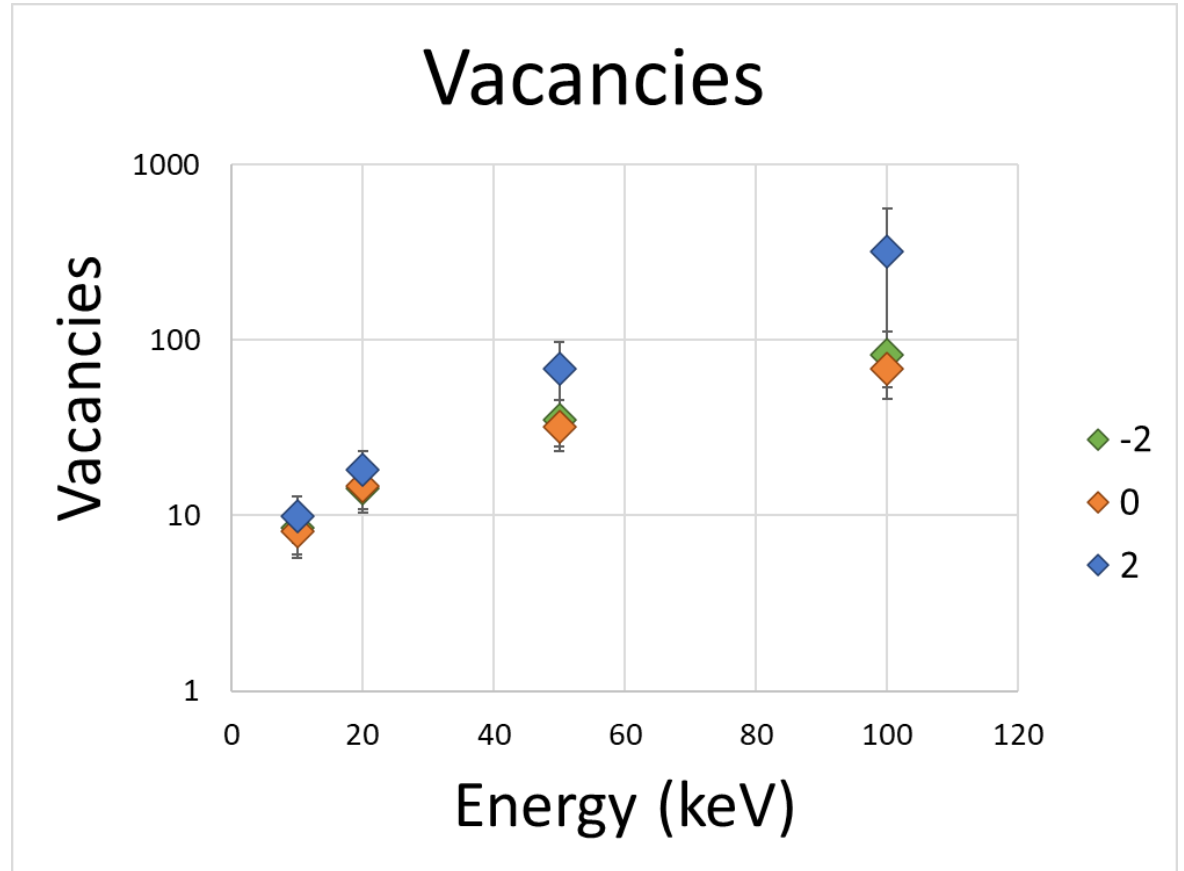
Cumulative cascade damage

- After 1000 consecutive 10 keV cascades in pre-damaged cell (2M atoms)
- More point defects, less dislocations for increasing strain



Individual cascade damage

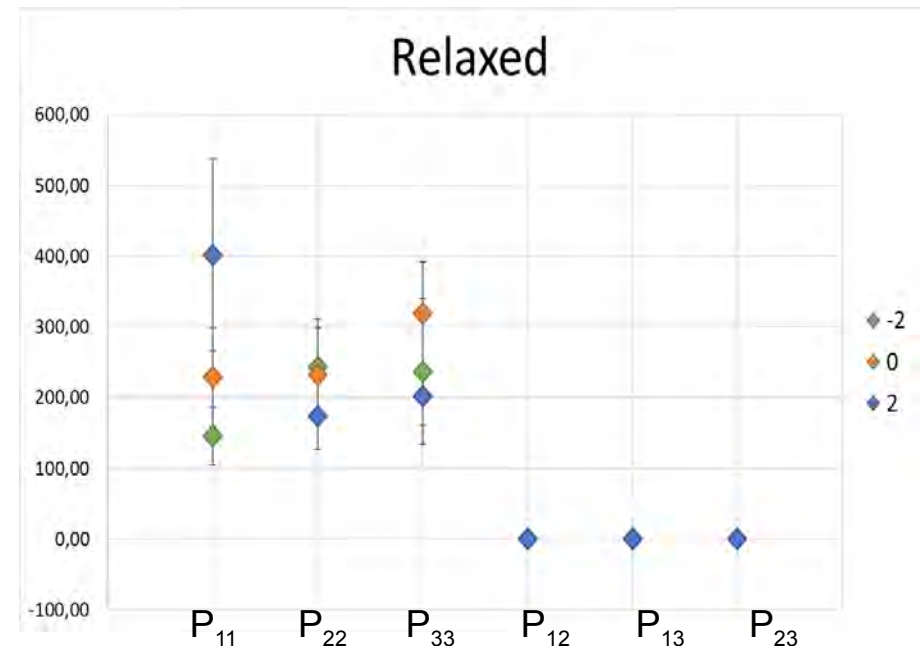
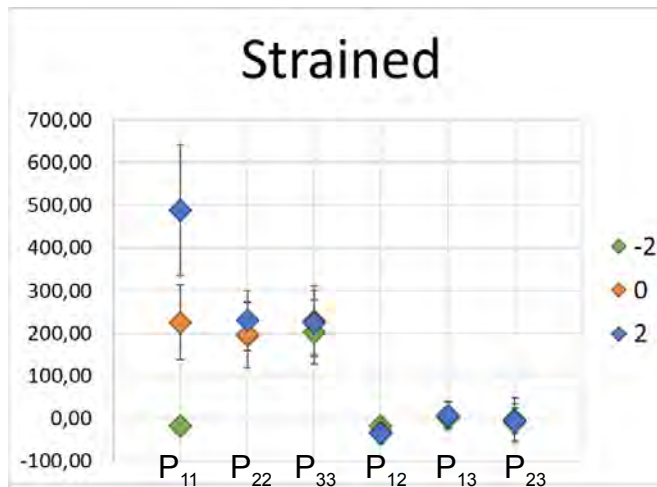
- 100 individual cascades simulated in a perfect monocrystal with 10 keV, 20 keV and 50 keV PKA energies, and 15 individual cascades for 100 keV PKA energy.
- Crystals were strained along $\langle 111 \rangle$ at -2% and 2% prior to cascades



Dipole elastic tensors

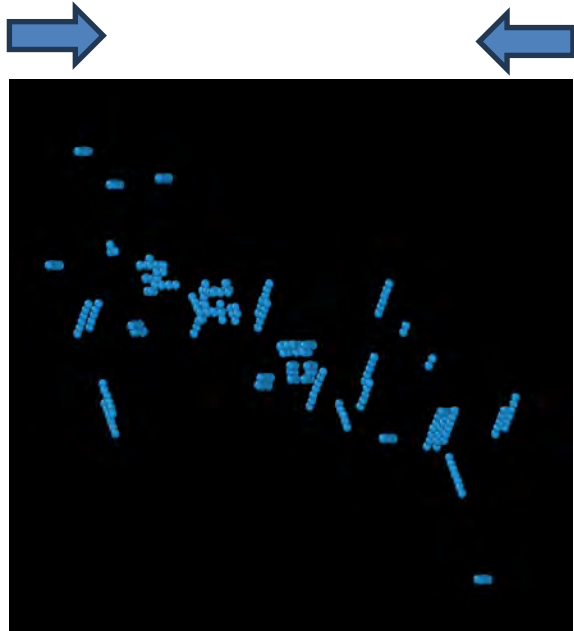
- Minimizing the energy of the cell with fixed volume
- Computing the pressure in the cell
- With the volume of the cell, it gives the dipole elastic tensor
- Useful for using it in FEM simulation afterwards

- Relaxing the cell in NPT to have no pressure at the boundaries
- Computing the relaxation volume
- With the elastic constant of the material, it gives the dipole elastic tensor

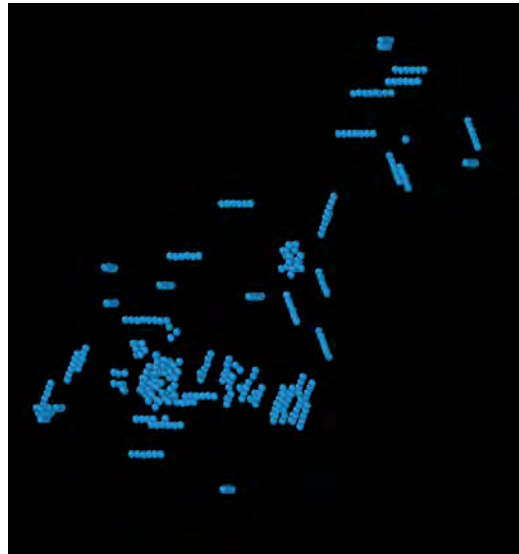


Crowdion alignment

- Polarization effects appear due to alignment of crowdion defects according to external strain



2% compression



No strain



2% traction

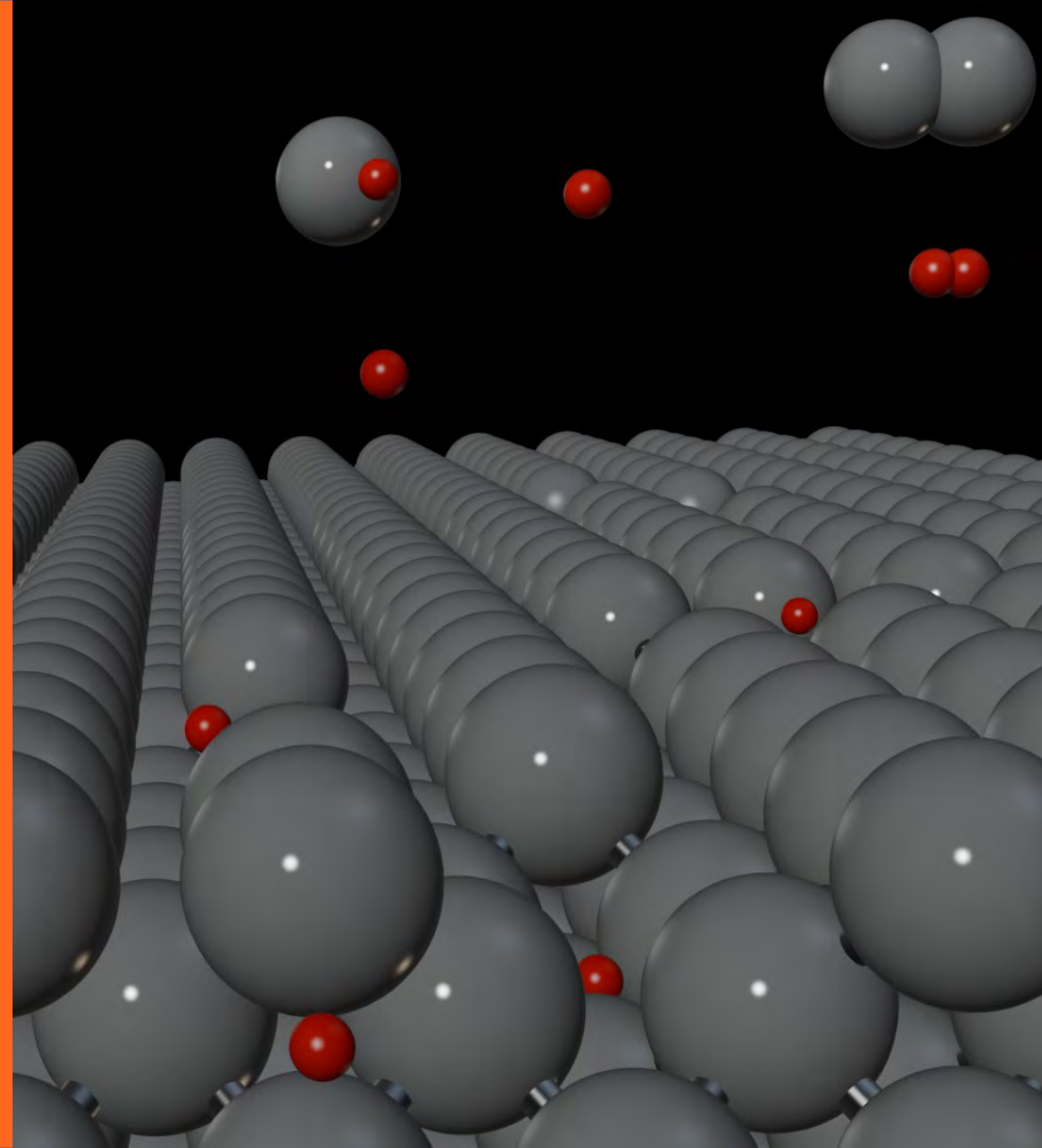
Sputtering and reflection from Be-H/D/T surfaces



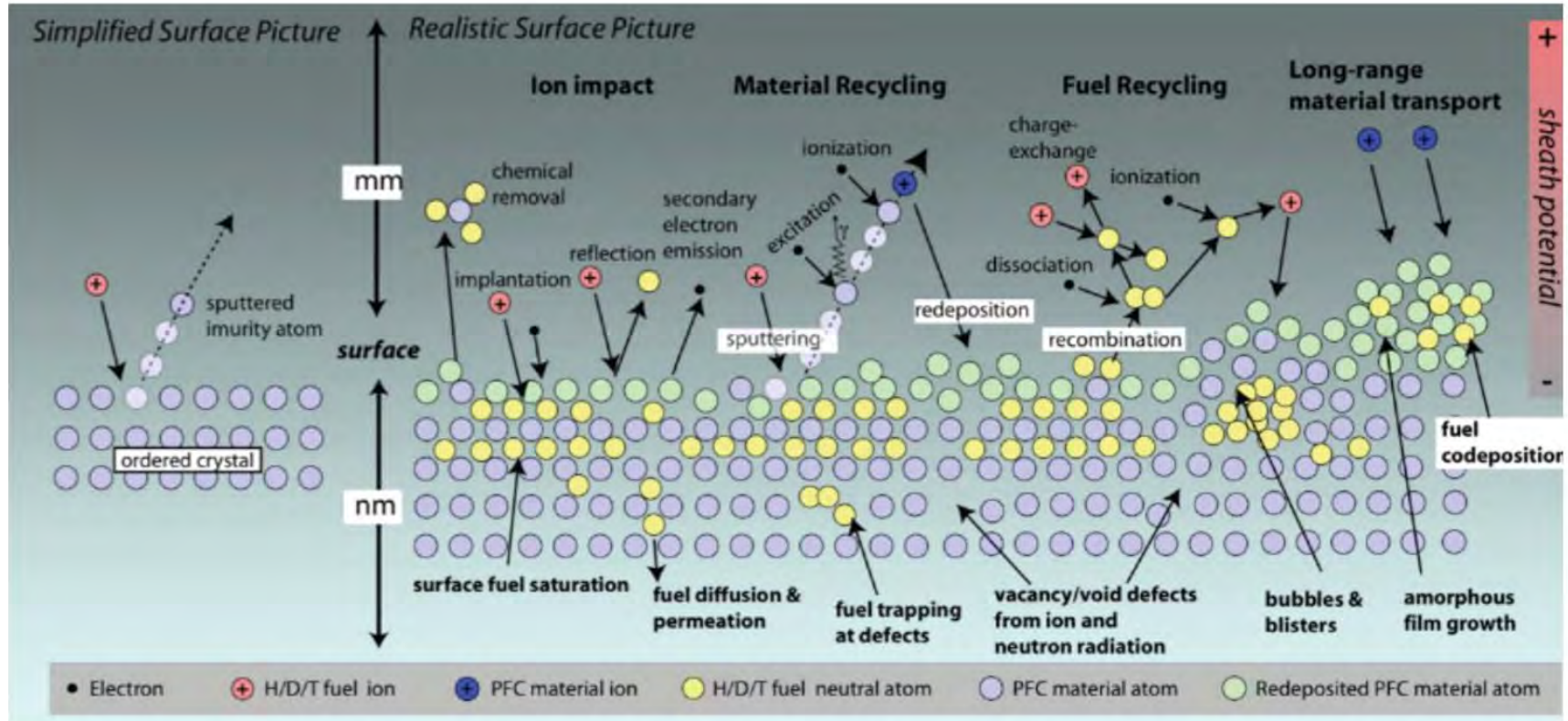
Nima Fakhrai Mofrad



Aalto University
School of Science



Plasma-surface interactions

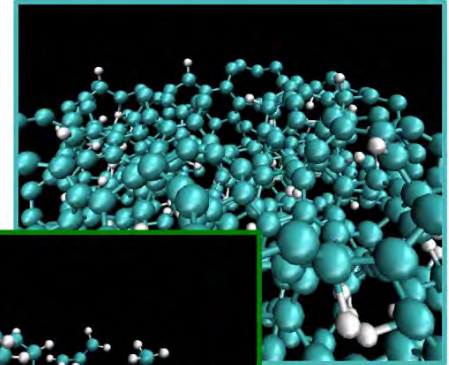


Chemical effects on sputtering

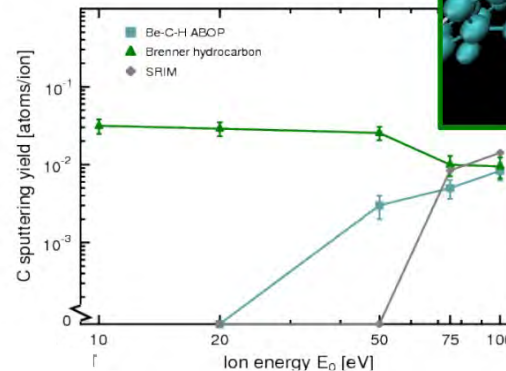
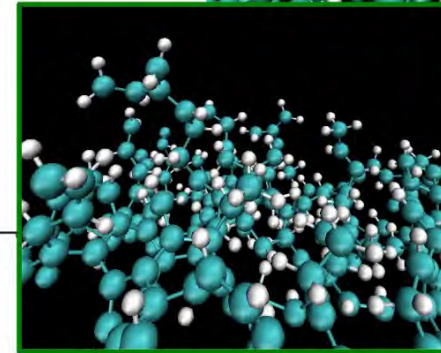
- Physical sputtering fairly simple to model
- Binary collision approximation (BCA) methods (e.g. with SRIM, SDTrimSP) can be used in many cases
- But, BCA breaks down
 - For low velocities (bonding, chemical effects, swift chemical sputtering)
 - Where crystal structure and many-body interactions matter, e.g. channeling

Potentials

Without bond-conjugation terms,
after 2001 impacts at 10 eV



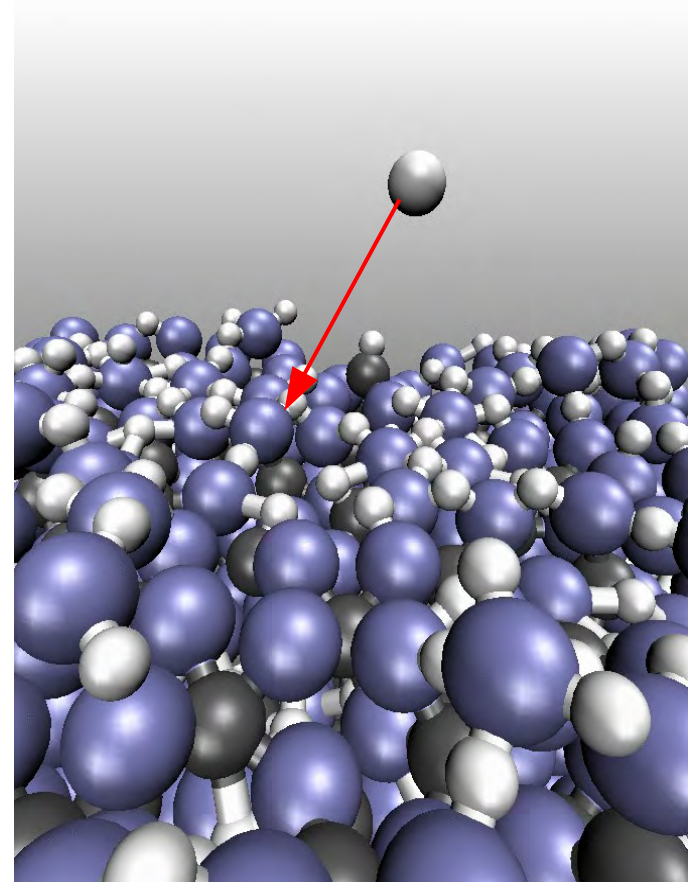
With bond-conjugation terms,
after 1091 impacts at 10 eV



Expected levels of C sputtering seen
only with bond-conjugation terms

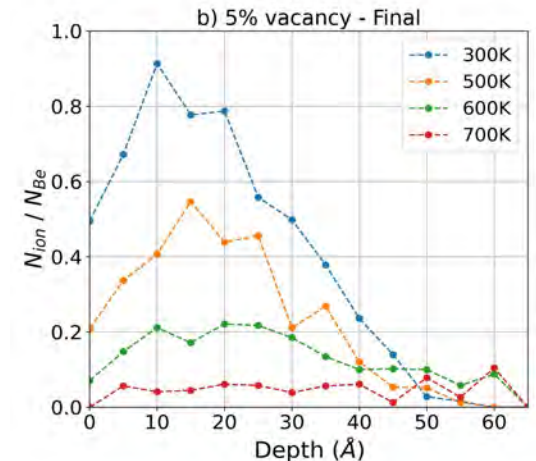
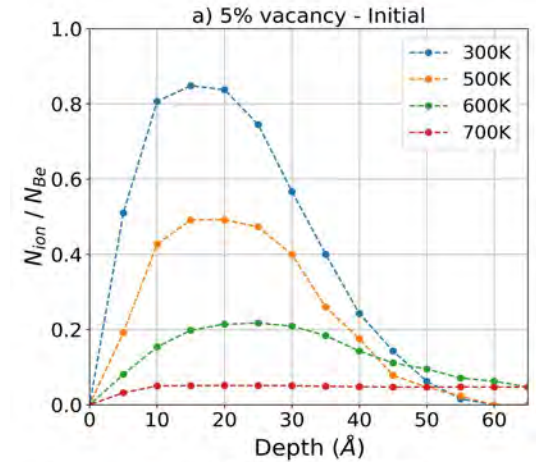
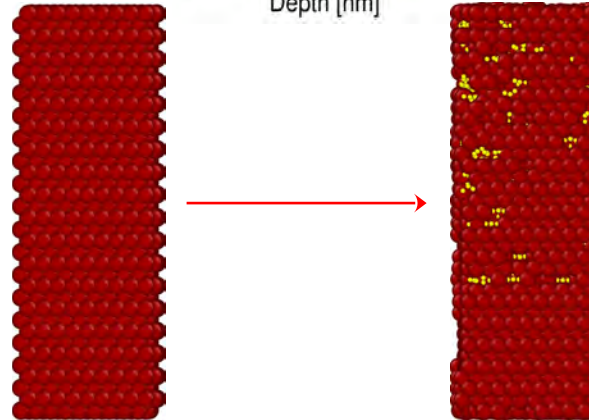
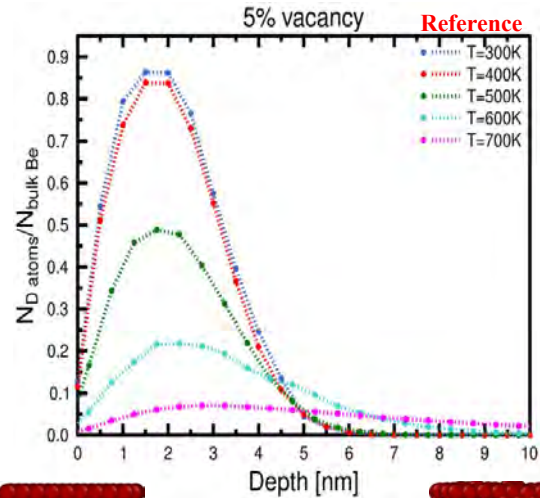
Sputtering with molecular dynamics

- Molecular dynamics can account for
 - Crystal structure, defect configurations, impurity content
 - Many-body interactions
 - Chemical effects of bonding on the level of the interatomic potential
- Initiate an atom (“ion”) above the surface, beyond the interaction range
 - Desired initial kinetic energy, impact direction
 - All interactions accounted for, integration of equations of motion
 - Excess energy removed via thermostat on borders of cell
- Follow full dynamics until impact event is over
 - Caveat: time scale ~ps
 - No time for diffusion
 - No time for thermally driven outgassing



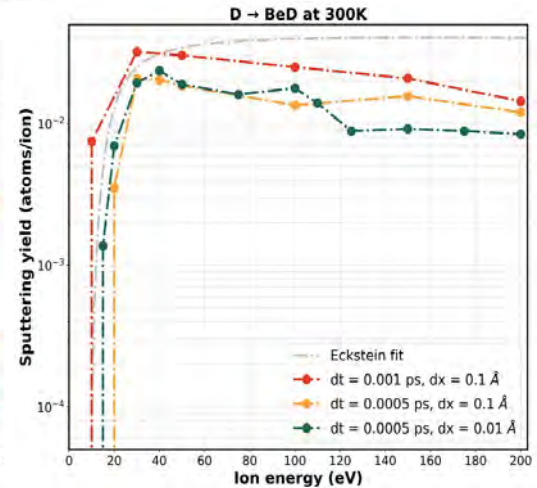
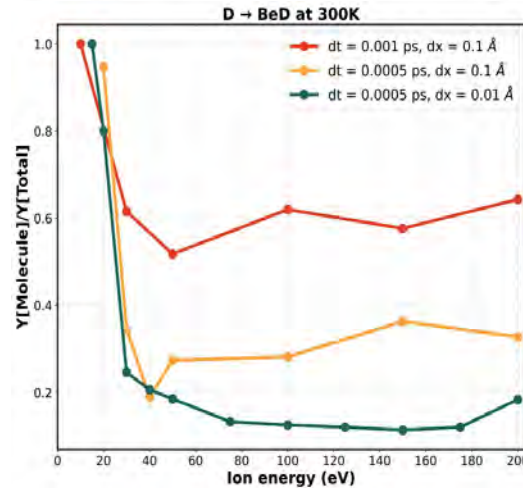
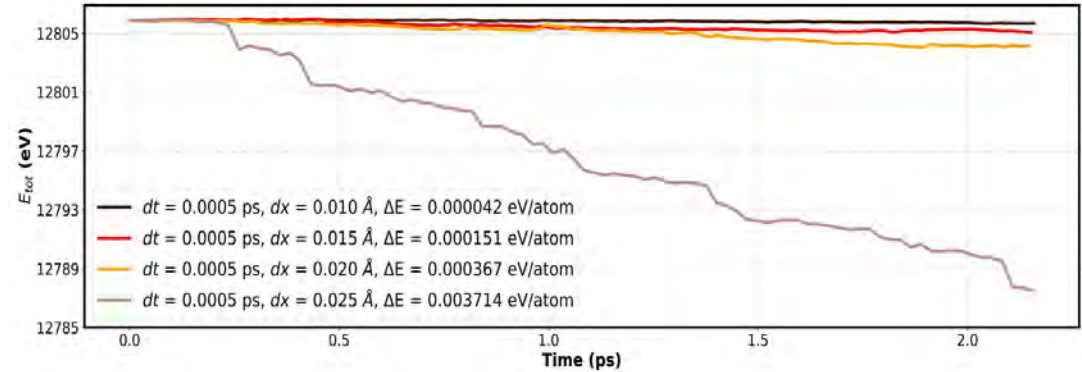
Simulation cells

- Be structures were initially loaded with H/D/T to set up a pre-existing concentration at different temperatures, based on the OKMC predictions of Safi et al. [6].
- Method
 - 5% of Be atoms were removed randomly to create vacancies
 - At each depth range, a certain number of vacancies were selected and 5 ions were inserted in each to obtain the initial distributions.
 - The cells were equilibrated and the final density profiles were obtained.



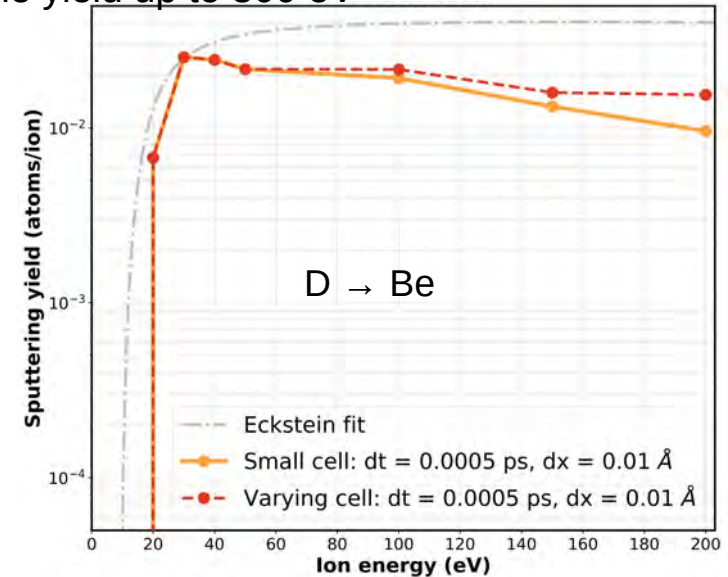
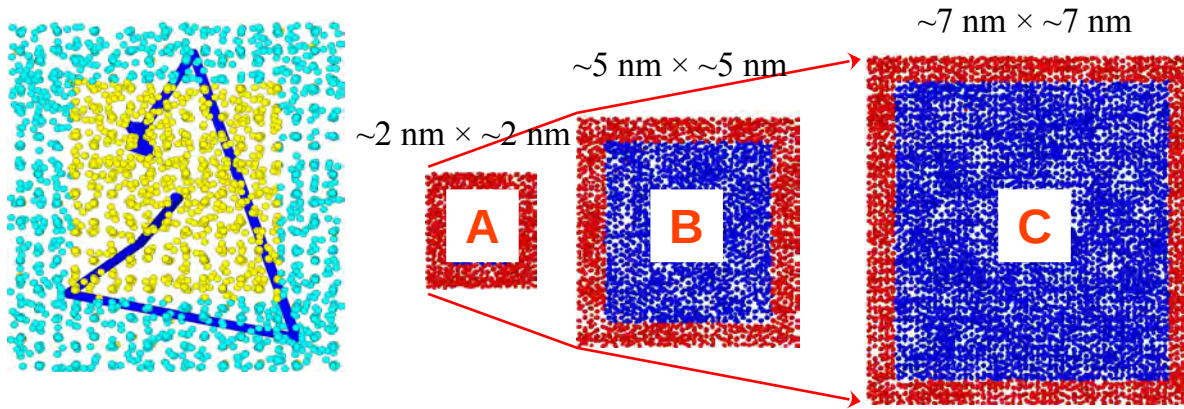
Integration time step

- H isotopes are very light, hence dynamics are very fast
- Accurate integration of equations of motion requires care
- Time step criteria: maximum allowed dt (fs) and dx (Å)
 - 0.5 fs in itself is not sufficient, but setting a maximum allowed time step to much smaller makes simulations incredibly slow
 - Adjusting the max dt has less impact on computational efficiency, but large effect on energy conservation and clear impact on predictions



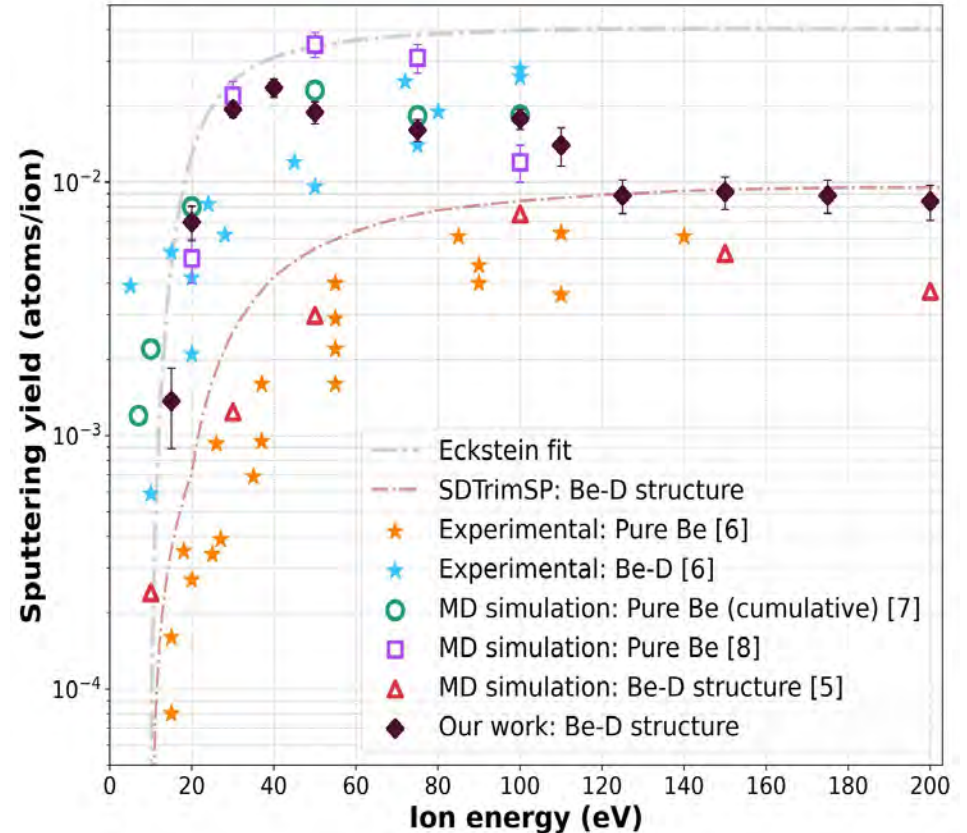
Cell size

- H/D/T ions can travel quite far in lateral directions beneath the top atom layer, and can cause sputtering far from the initial impact point
- If the cell is too small, this may happen in the border region, and sputtering would be inhibited due to the velocity scaling of the thermostat
- With a large enough cell size, we observe only minimal decrease in the yield up to 300 eV
 - Normal incidence: A: $E \leq 40$ eV; B: $50 \leq E \leq 100$ eV; C: $E \geq 150$ eV
 - Angled incidence: B: $E \leq 50$ eV, C: $E > 50$ eV



Sputtering yields

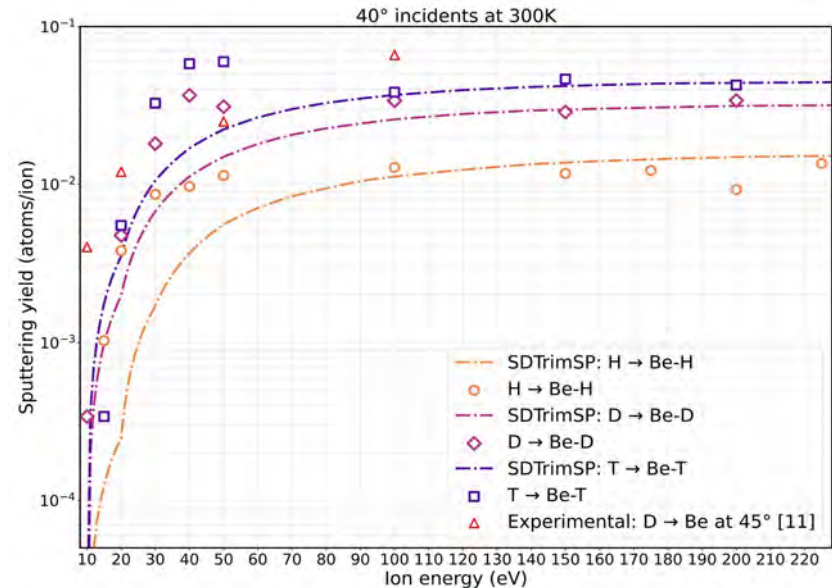
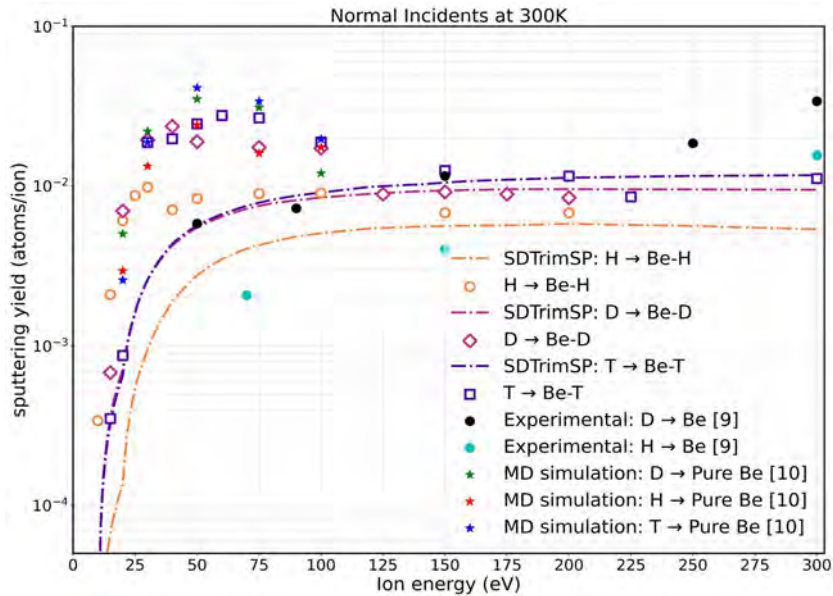
- Sputtering yield defined as the number of Be atoms leaving the surface divided by the total number of impacts
- The figure represents the total sputtering yield at 300K for normal incidence
- Good agreement with the experimental values for Be with D present in the structure (blue stars)
- No decreasing trend in the yield is predicted for impact energies higher than 100 eV



Isotope effect

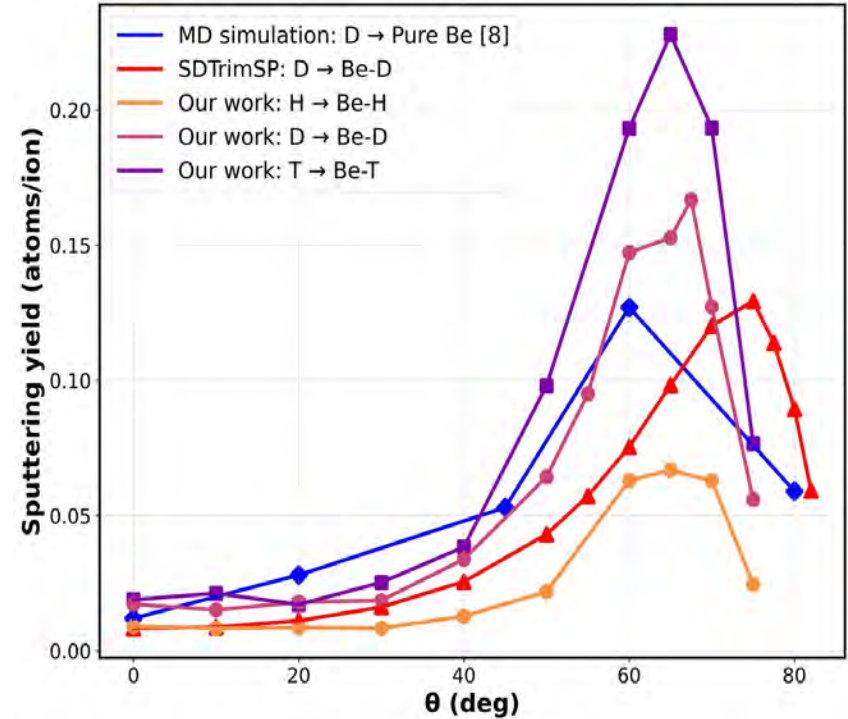
- In general, increasing the isotope mass will result in an increase in the sputtering yield

- Good agreement with SDTrimSP results at higher impact energies
- Below about 100 eV, the accuracy of MD is needed



Impact angle dependence

- Increasing the impact angle from 0° to $\sim 65^\circ$ increases the sputtering yield
- Further increments will result in a sharp decrease of the sputtering yield
- Same behavior is observed for all isotopes, with only difference being the magnitude of the yield
- Compared to SDTrimSP data we get higher yield values, with the maxima at lower angles followed by a sharper decrease



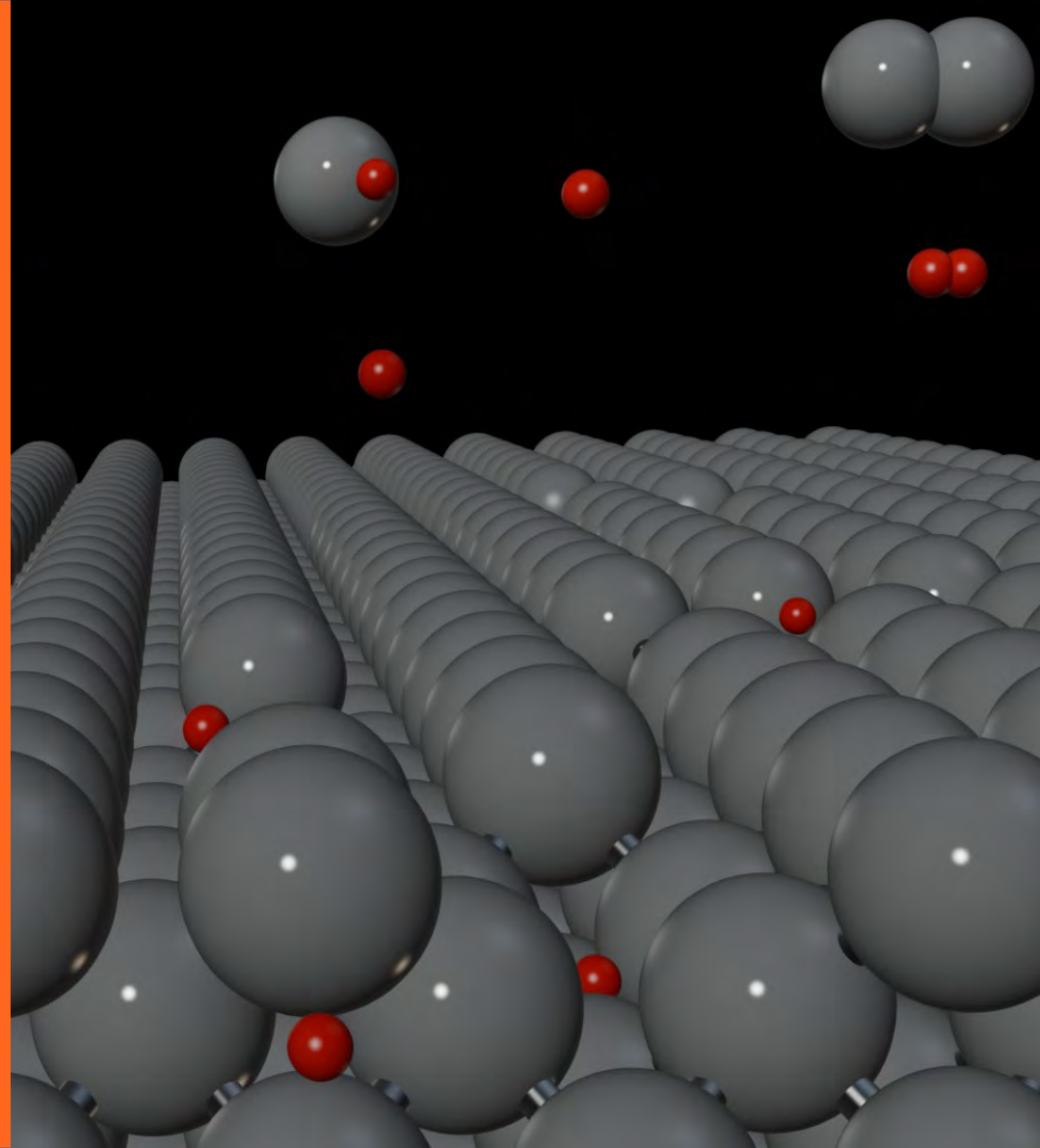
Nitrogen reflection from W-N surfaces



Akseli Aro and Nima Fakhrai Mofrad



Aalto University
School of Science



Context and motivation

- Nitrogen impurity injection used in ASDEX Upgrade and JET tokamaks to improve plasma performance
- To model N transport in the divertor region (carried out by the fusion group at Aalto), knowledge of interactions of N ions with the surface is needed
 - Reflection coefficients, atomic or molecular species, energy distributions
- High impact angles and low energies expected in the divertor region
 - Median impact energy around 8 eV, tail up to 150 eV
 - A multiply charged N ion expected to impact the surface at around 60 degree angle

Simulation set-up

- SIMULATION CELL

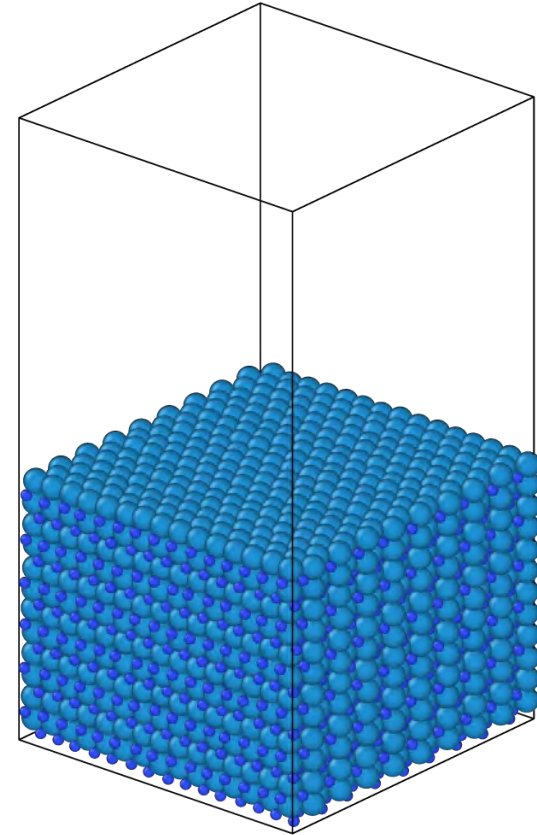
- We assume a 1:1 ratio of W and N
- NiAs crystal structure, lowest energy configuration of WN according to potential
- size 6480 atoms or 44 by 45 by 35 Å

- BASE SIMULATION

- 30 ps NPT relaxation at 500K
- Open surfaces normal to z
- 30 ps NVT relaxation at 500K
- Start irradiation with N ions

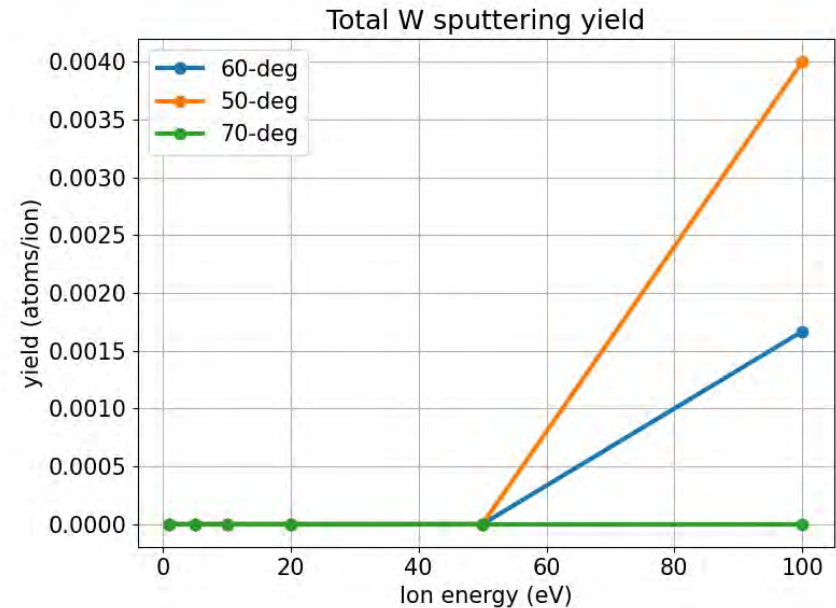
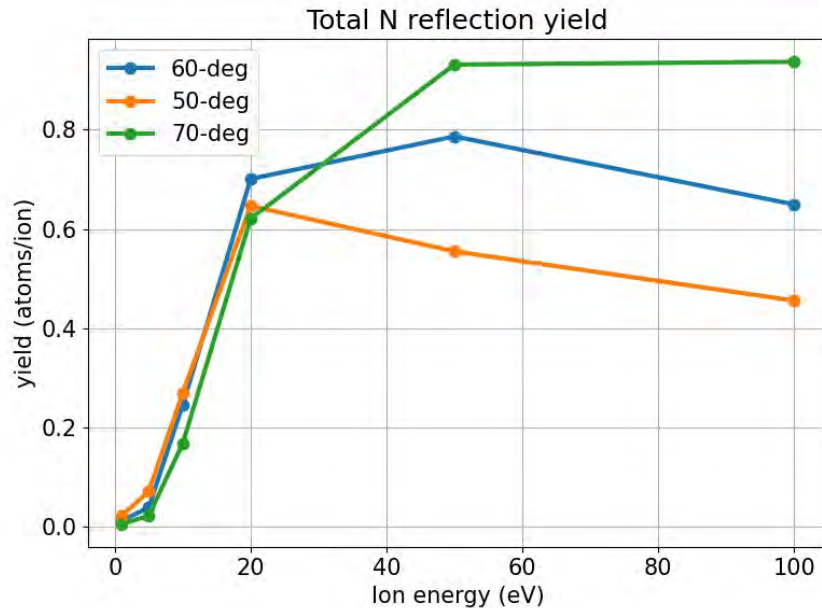
- IMPACTS

- 50, 60, 70 degree incident angles
- Six different energies per angle (1,5,10,20,50,100 eV)
- 3000 simulations per ion energy



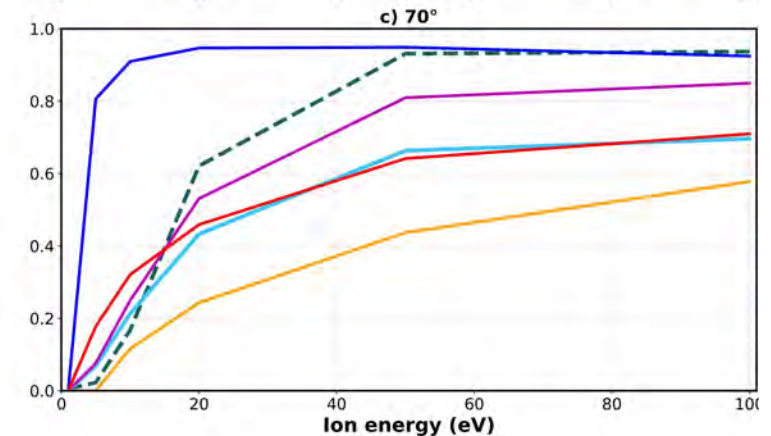
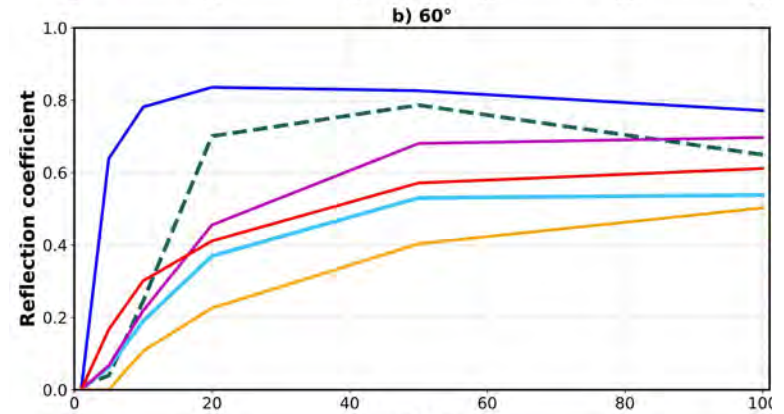
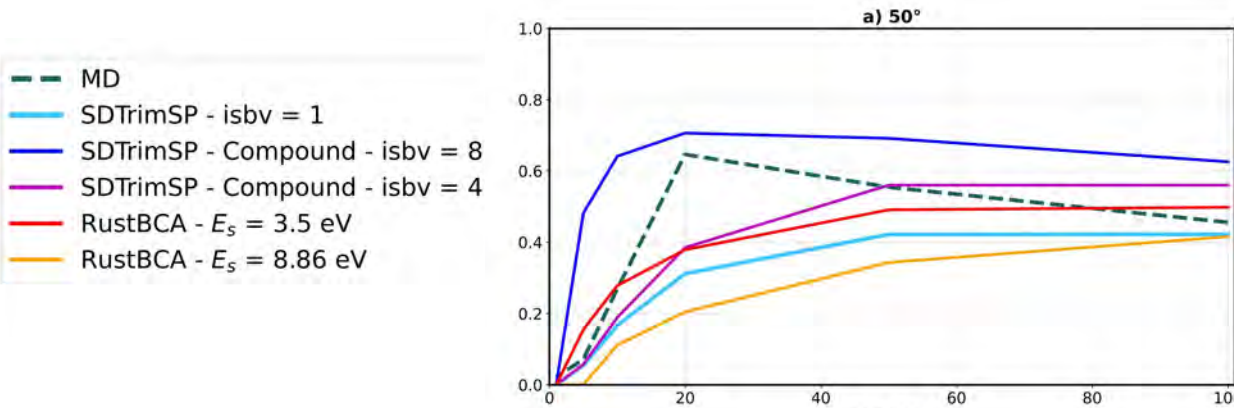
Reflection and sputtering

- Reflection probability increases with increasing impact angle for higher impact energies, while sputtering decreases with increasing angle



N reflection for glancing incidence

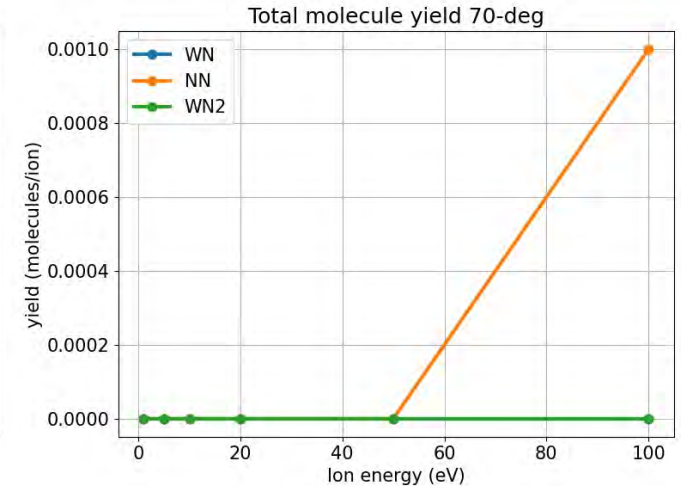
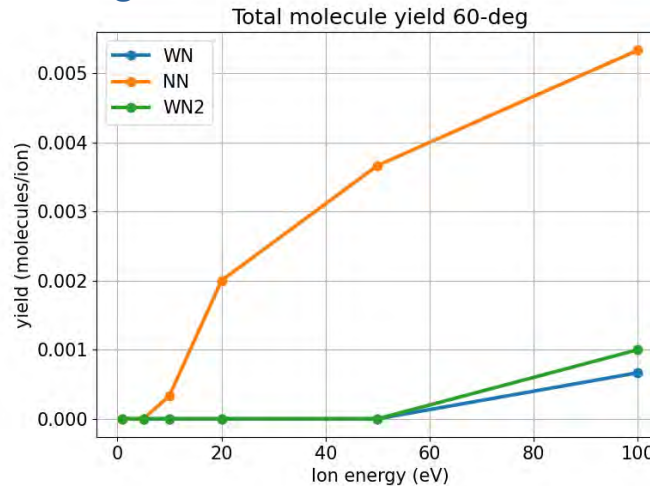
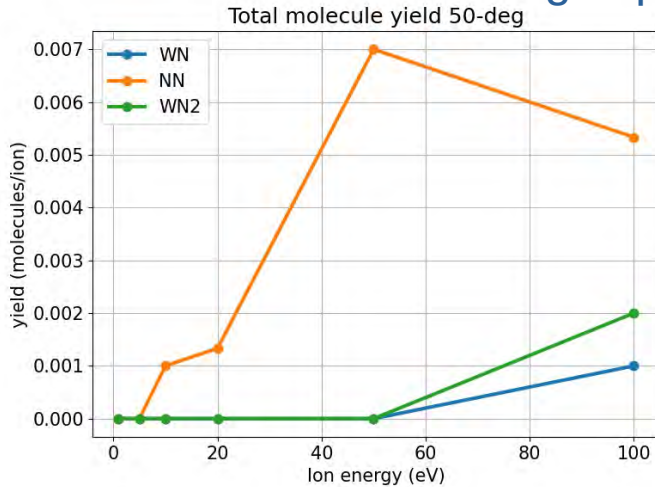
- MD shows the point of maximum reflection moving towards higher ion energies the higher the impact angle
- BCA does not capture this behaviour
- Uncertainties in the surface binding energy model leads to large differences in predictions from SDTrimSP
 - None correspond well to the MD predictions for low energies



Molecular yield

- Molecular N_2 yields decrease for increasing impact angle
- At 100 eV one begins to see WN_x molecules

Increasing impact angle

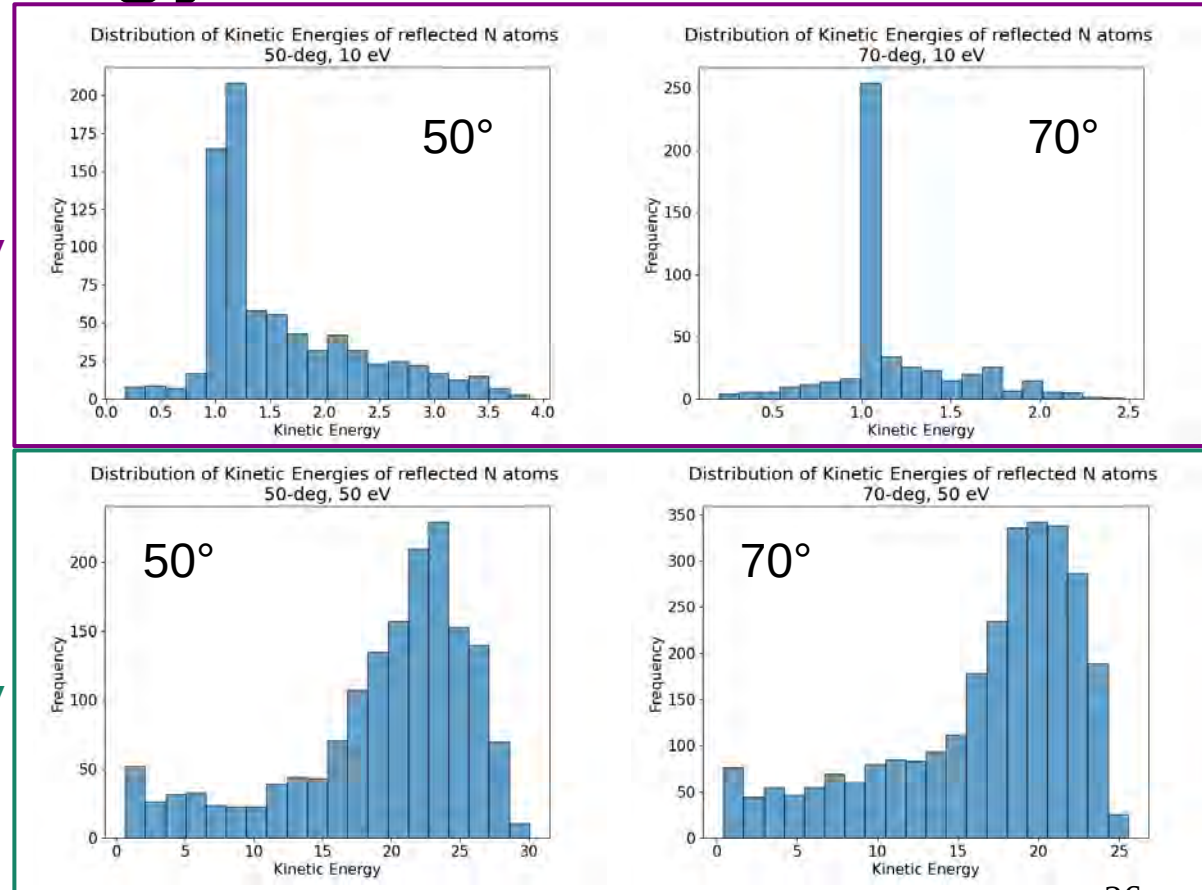


Kinetic energy distributions

- Kinetic energy distribution of reflected N atoms not strongly dependent on impact angle
- Distributions are skewed differently for different impact energies
 - For 10 eV, most ions retain only 10% of their kinetic energy, with a tail heavier towards higher energies
 - For 50 eV, most ions retain about 40% of their kinetic energy, with a tail towards lower energies

10 eV

50 eV



Conclusions

- Cascade damage is sensitive not only to the existing microstructure, but also to external loading conditions
- Chemical effects in Be-H/D/T systems results in peaks for sputtering yields at low energies
 - Accurate simulations with light ions requires care in setting the time step
 - For higher energy ions, fairly large cell sizes are needed
- At higher energies, sputtering from Be-H/D/T systems predicted by MD agrees well with SDTrimSP
- Reflection yields (of N from W-N surfaces) at low energies is sensitive to bonding effects not well captured by the “surface binding energy” of BCA models

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Thank you!



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EUROfusion