WP PWIE SP D:
Activities 2022, Outlook

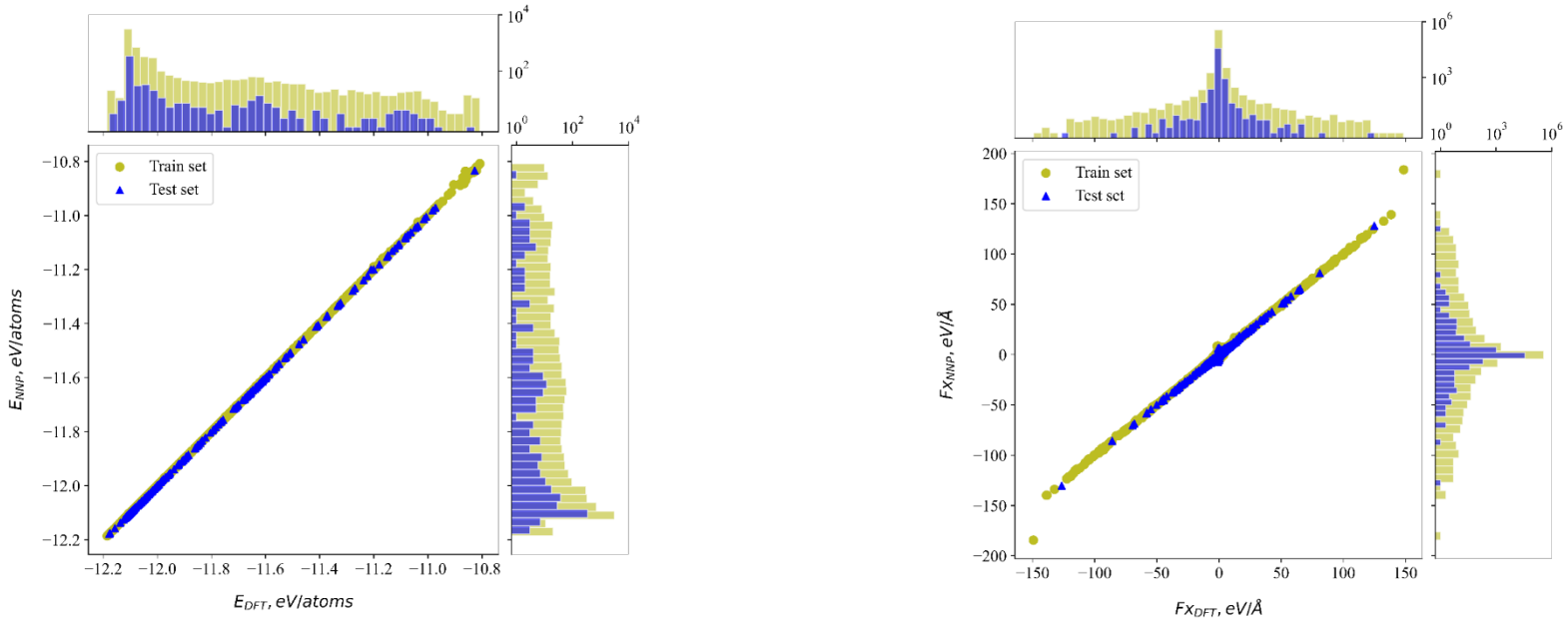
Michael Probst

Shokirbek Shermukhamedov,
Jose Romero

Austrian Academy of Sciences (OEAW)
Institute of Ion Physics, University of Innsbruck

MD Method

- MD of plasma-surface interaction by ML-Potential Energy Functions
- Speed-up of density functional (DFT) calculations by transferring the system information to an analytical function without loss of accuracy. In our case a NN is used. There are now many alternatives.

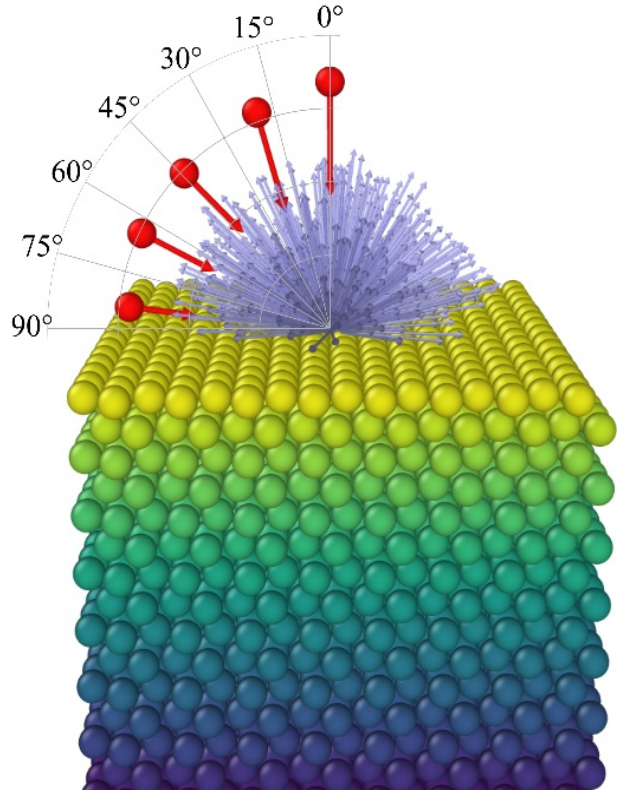


Two-dimensional histograms of DFT-calculated and NNP-predicted atomic energies (left) and forces (right).

*L. Chen, et al., RSC Advances 10(8) (2020) 4293-4299

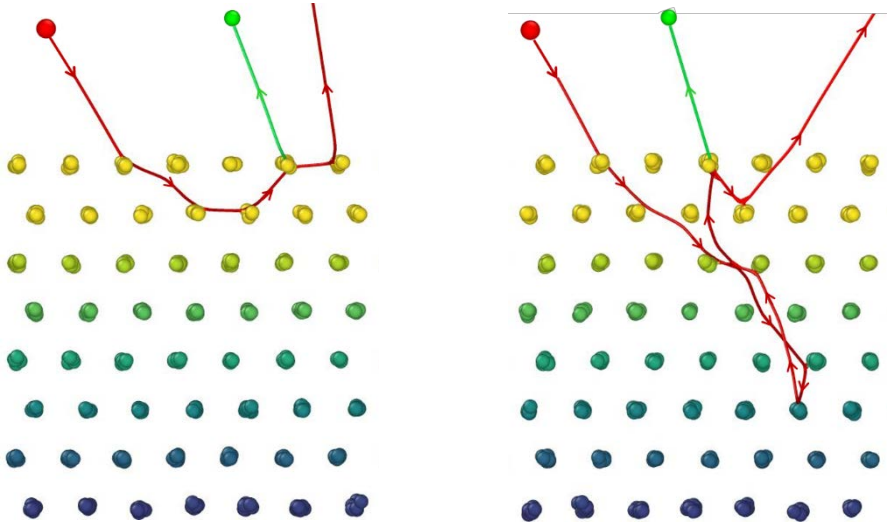
System 1: Be/D and Be/T

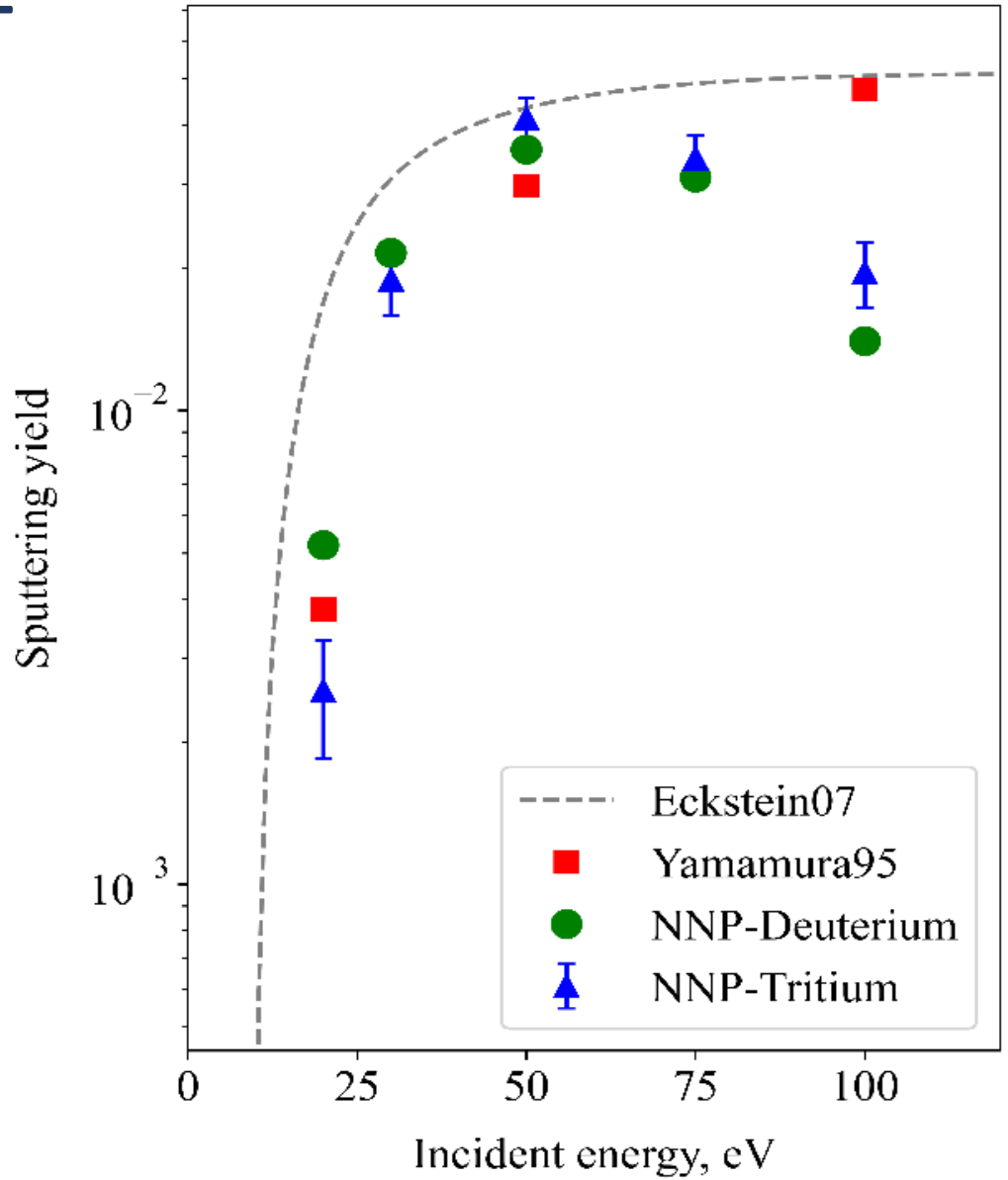
- Be / D and Be / T : Be surfaces by 10, 20, 30, 50, 75, 100 eV D and T atoms;
- NVE ensemble;
- Non-cumulative simulations;
- For each impact 2000 (5000) MD simulations are performed;
- The sputtering angle φ is defined as the angle between the velocity vector of the outgoing particle and the surface normal;
- Used: LAMMPS, n2p2 Behler-Parinello type High Dimensional Neural Networks Potential (BPHDNNP); our Python analysis codes



1.A Sputtering yields for D and T

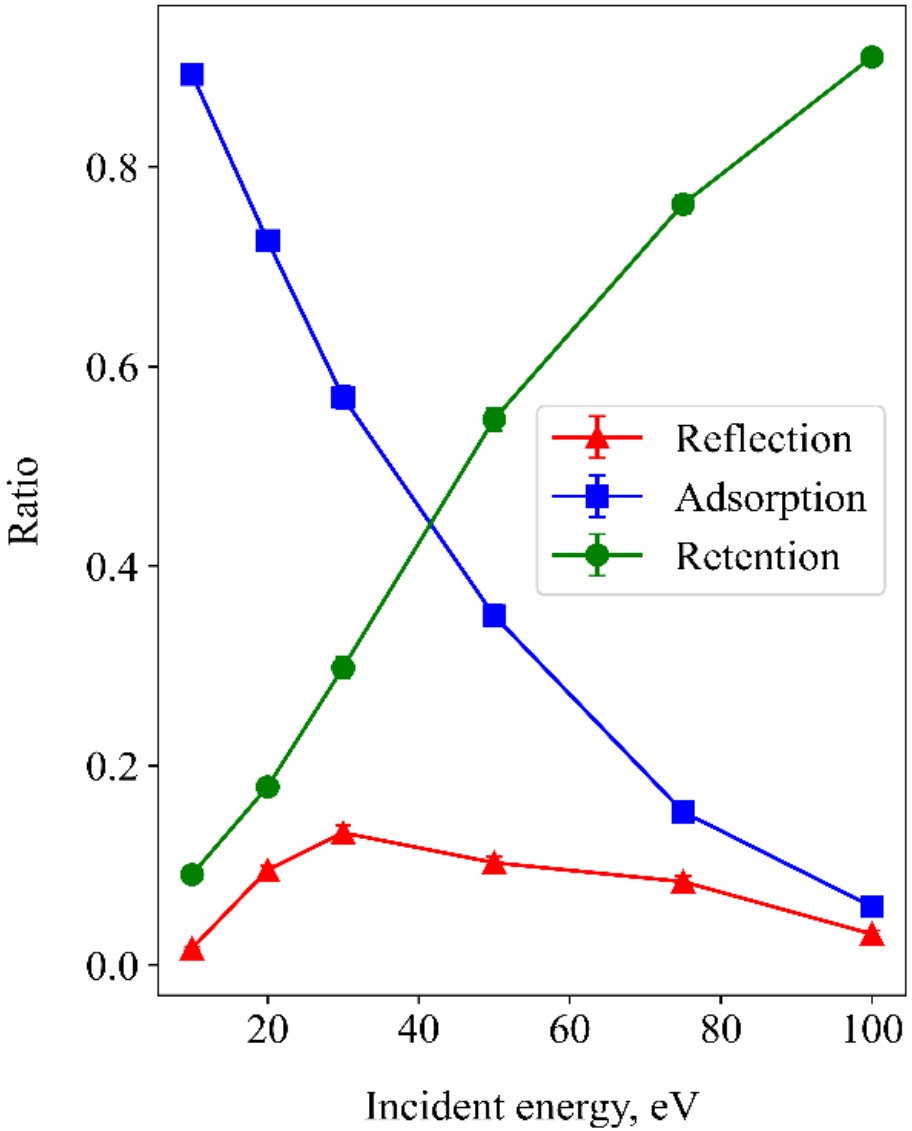
- The sputtering yields for D and T are very similar for a certain incident kinetic energy (=the lower initial velocity compensates the effect of a higher mass).





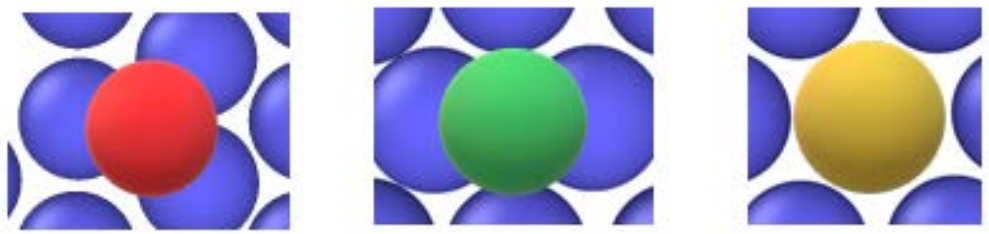
1.B Reflection, Retention and Adsorption

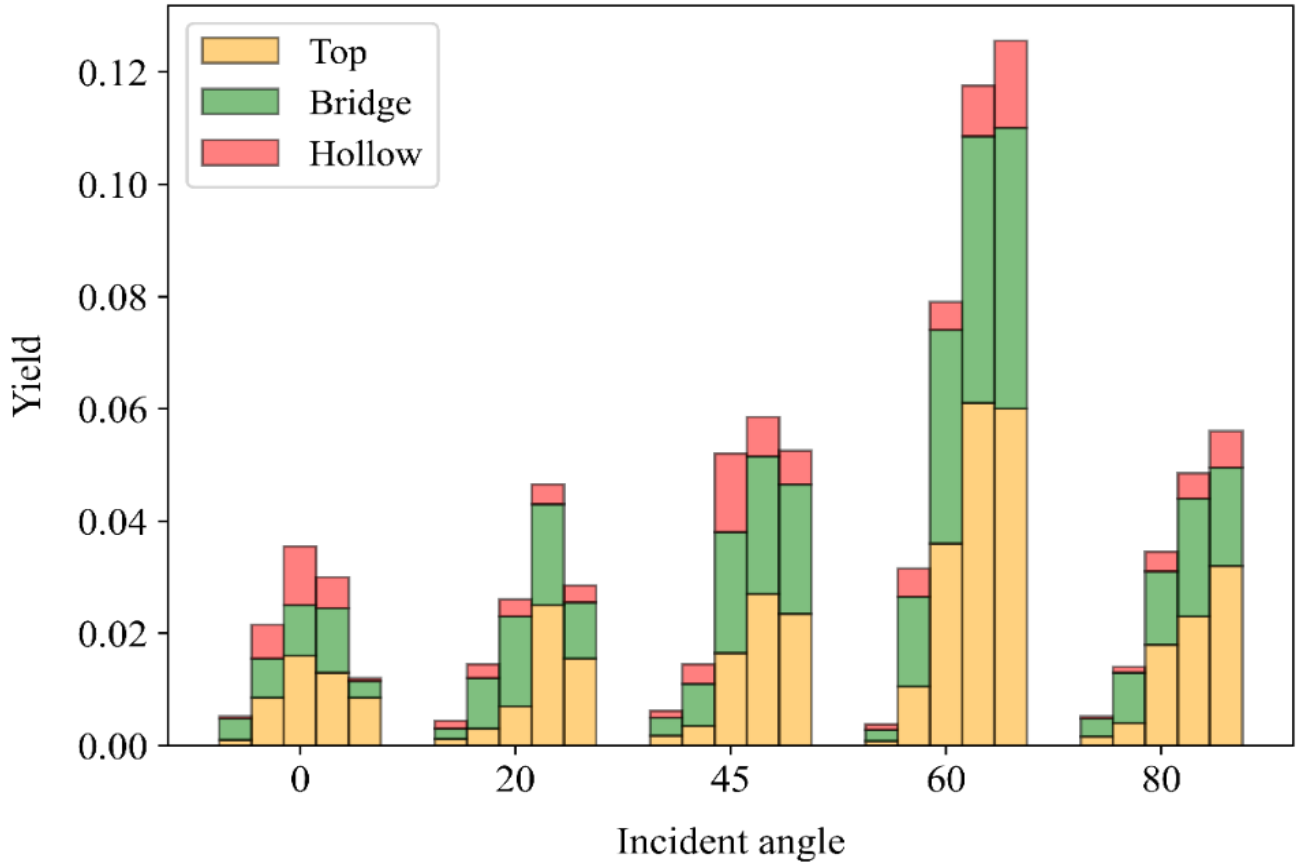
- The maximal reflection probability is found at energies between 30-50 eV.
- At energies higher than 40 eV reflection and retention ratio are ~equal.
- This behavior of T is also similar to that of D.



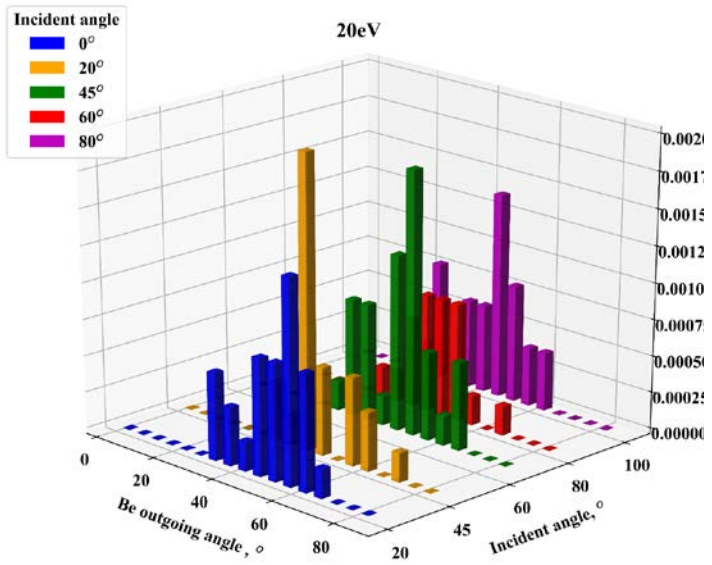
1.C Dependence on Impact Position

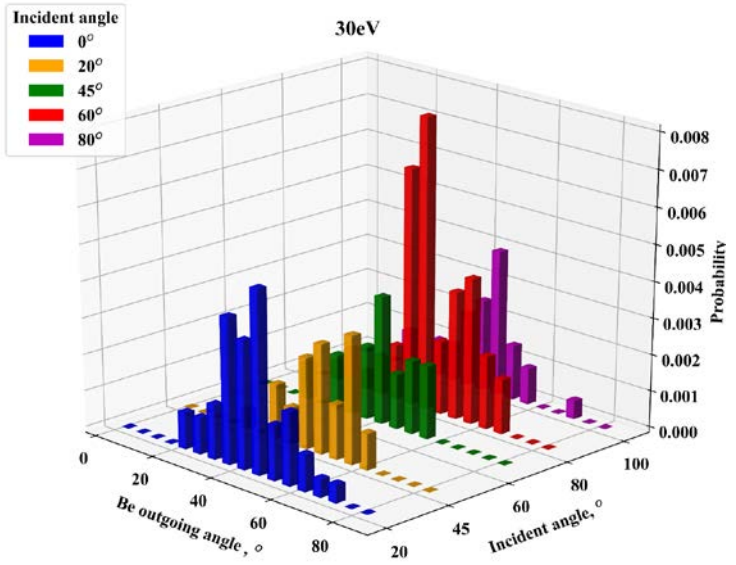
- ‘top’, ‘bridge’, ‘hollow’ position sites
- Hollows sputtering has smallest contribution to the total yield.
- Top and bridge are approximately equal.

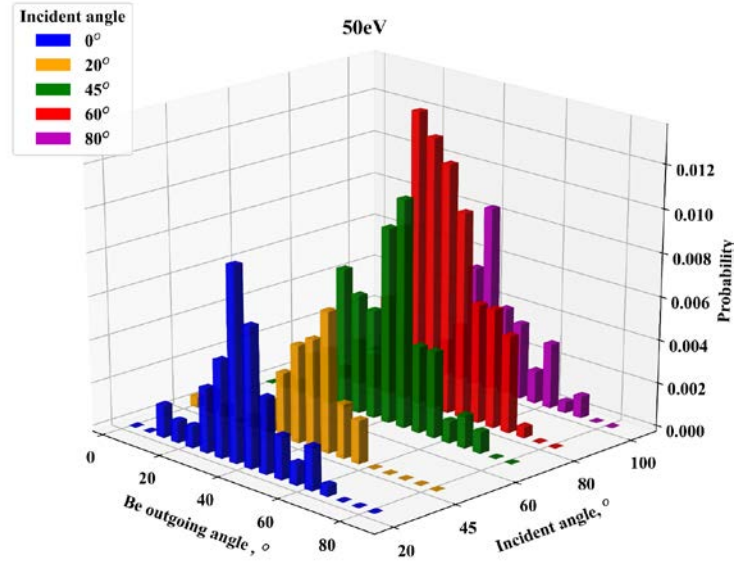


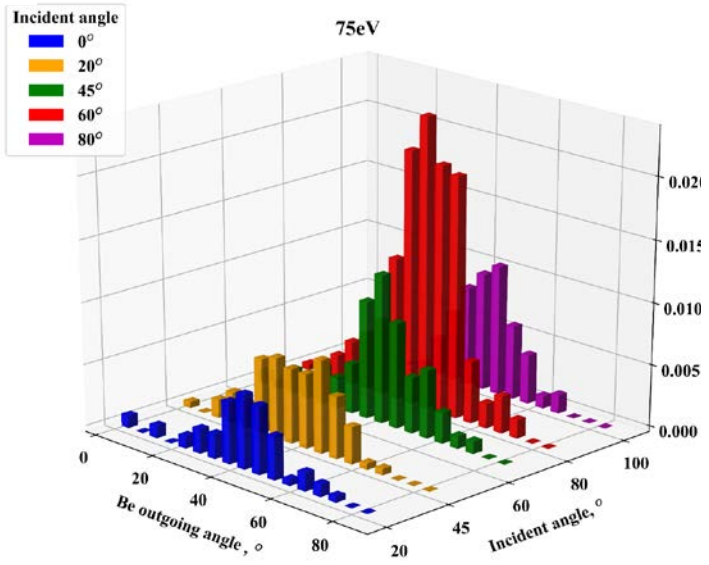


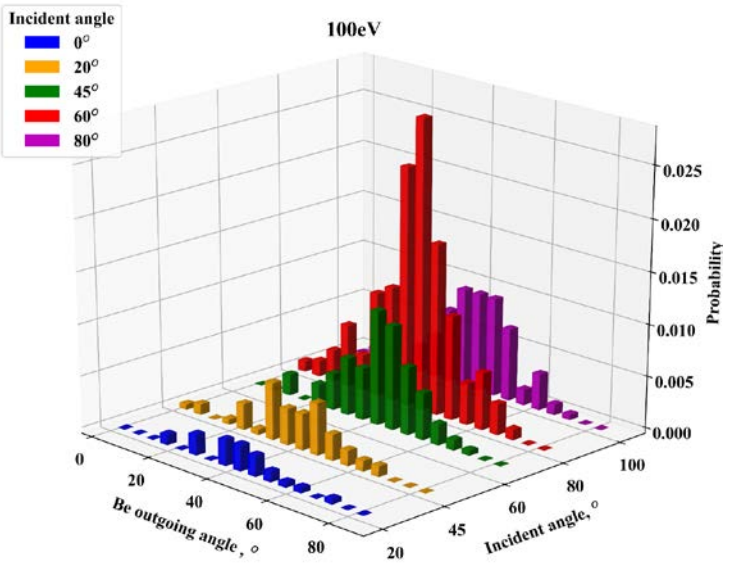
1E Be outgoing angle distributions











2A Energy Spectra of Sputtered Atoms

- Thompson propagated a formula the energy spectrum of sputtered atoms as a function of the incident energy:

$$Y(E) \sim \frac{E}{(E + E_{SB})^k}$$

- Falcone improved this formula to fit the incident energy dependence of the of the energy spectrum of *atoms sputtered from heavy target materials by low-energy light-ion bombardment*:

$$Y(E_0, E) \sim \frac{E}{(E + E_{SB})^k} ln \frac{\gamma E_0}{E + E_{SB}}$$

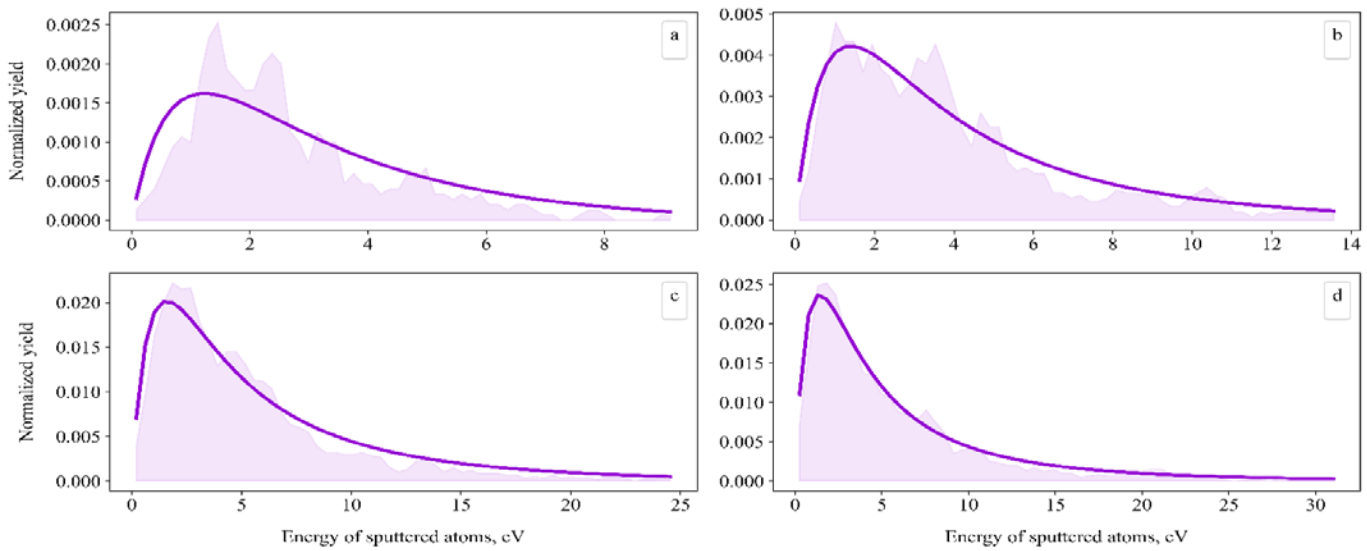
- E is the energies of sputtered atoms, E_{SB} is the surface binding energy of the target material and E_0 is the energy of incident atom. $\gamma = 4M_1M_2/(M_1 + M_2)^2$ where M_1 and M_2 are the masses of an incoming ion and a target atom. The value of k depends on the interaction potential for elastic collisions (k =3 in Thompson and k =2.5 for Falcone)

2A MD Results vs. Falcone formula:

Best values of k and E_{SB} determined by fitting.

Incoming energy, eV	*k*	E_{SB}, eV
30	3.83	4.58
50	3.56	4.43
75	2.98	3.93
100	3.11	3.55

The value used in BCA simulations is **3.38** eV
DFT value is **5.128** eV.

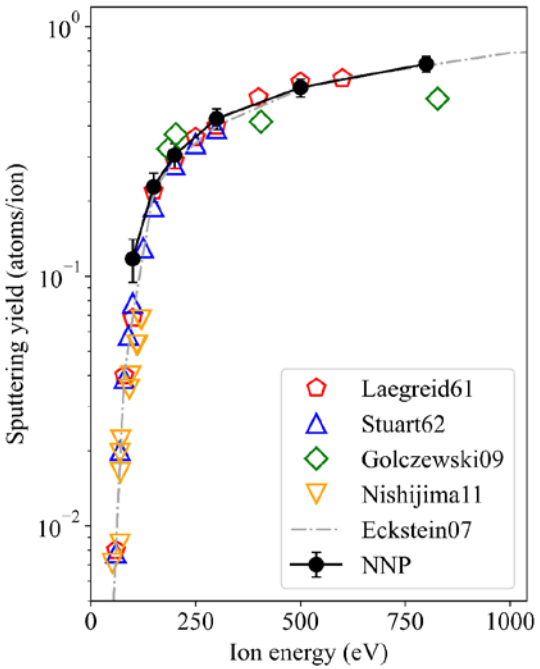


Result:

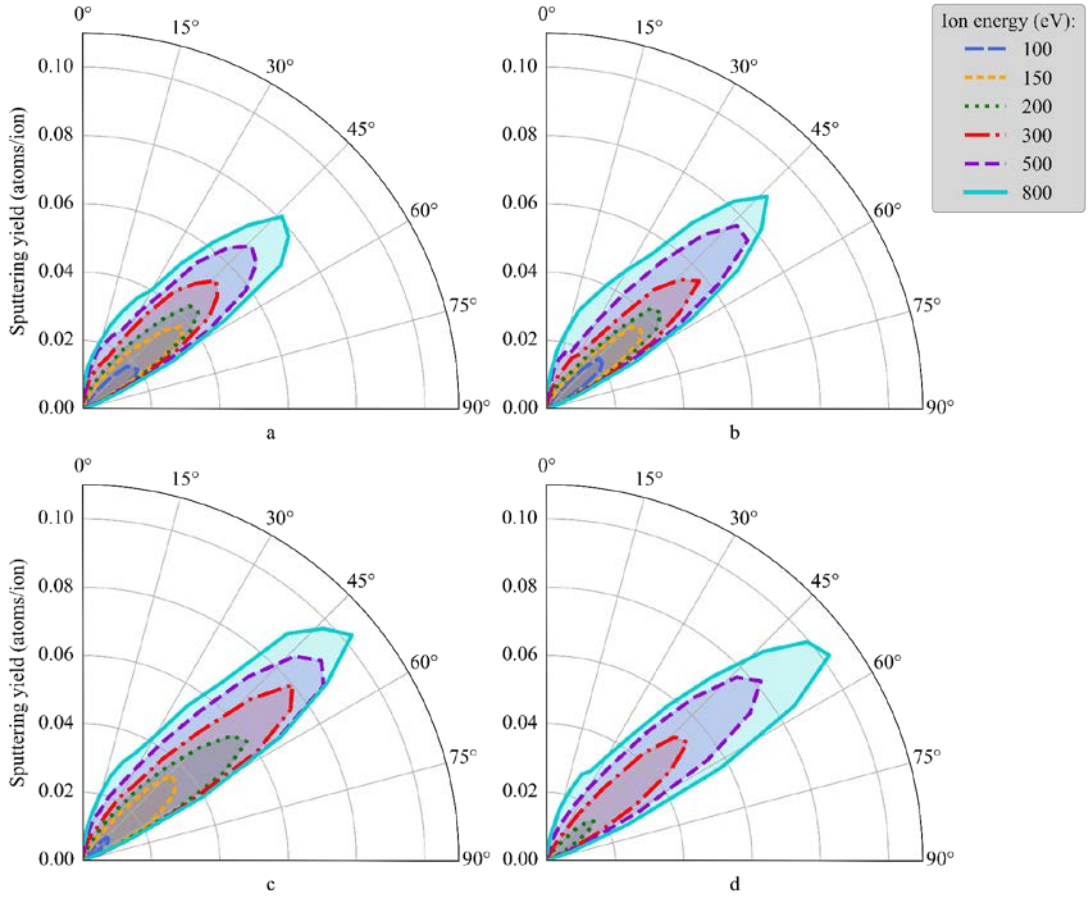
- **The energy distributions of sputtered atoms are reasonably reproduced by the Falcone energy spectrum.**
- **The surface binding energies estimated ('back-calculated') from the simulation are between 4.6 and 3.6 eV. There is a dependency on the impact energy.**

3A Impact of Ar on a W surface

Good agreement for sputtering



- **Analysis of angular distributions for sputtering:**
  Yields and angles of sputtered W atoms as a function of Ar incident energy (0° = surface normal (a), 20° (b), 40° (c) and 60° (d).

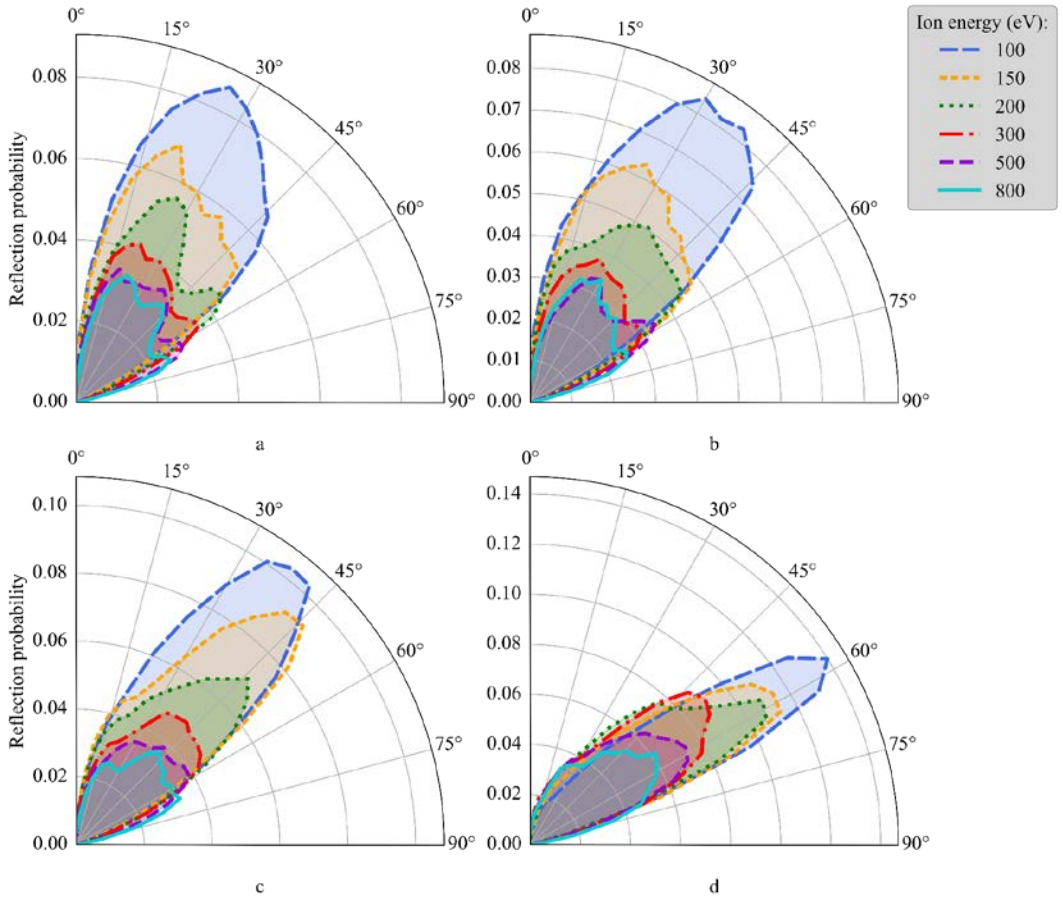


- **W atoms sputtered between 35-55°**
- **Not much energy dependence**

3B Impact of Ar on a W surface

- **The same for reflection: Angular distributions**

  Yields and angles of sputtered W atoms as a function of Ar incident energy (0° = surface normal (a), 20° (b), 40° (c) and 60° (d).

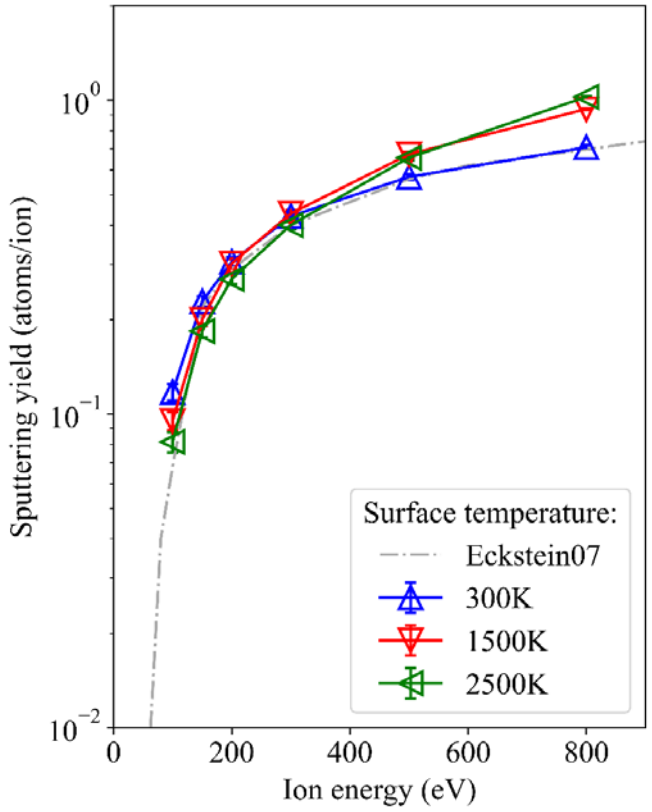


- **More dependence on incoming angle than for sputtering**
- **Broader than for sputtering**

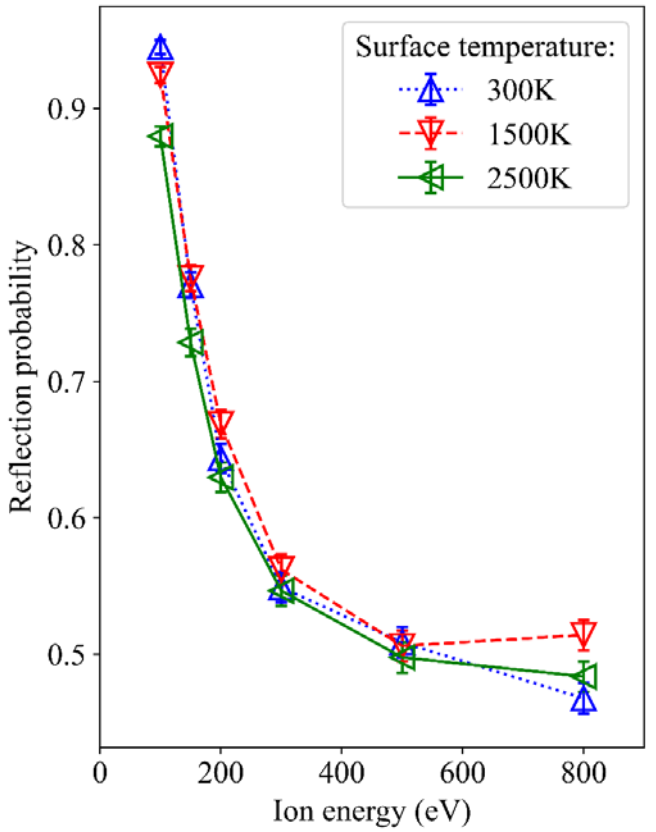
3 Only a small T-effect is found

300K, 1500K and 2500K

(a) Sputtering yields (b) and reflection probabilities (b)



(a)

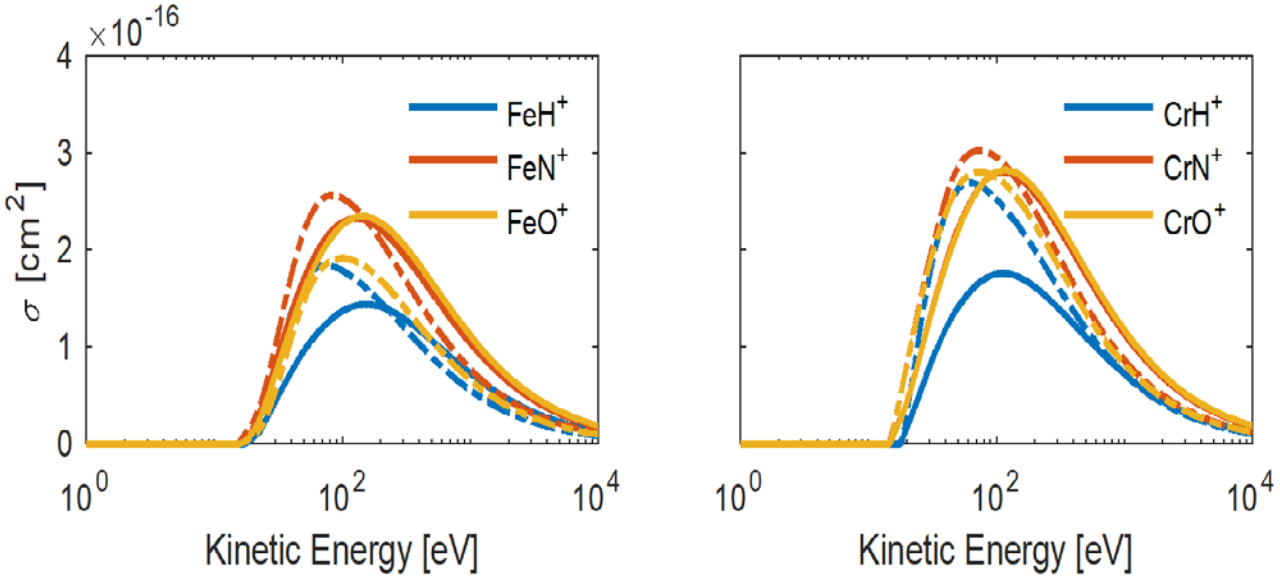


(b)

4A Electron-impact ionization cross sections

- EICS for neutral and ionic species of the mono-Hydrides, Nitrides and Oxides of Fe and Cr.
- Calculations with the DM and BEB methods.

- Total cross sections as function of the kinetic energy of an incident electron
- diatomic cations with Fe (left) and Cr (right)
- BEB (solid lines) and DM (dashed lines) methods.



Publications 2022

Be/D and Be/T:
Nucl. Fusion ***62*** *(2022) 066024,* DOI:10.1088/1741-4326/ac592a

Ar/W:
Eur. Phys. J. D (2022) 76:169, DOI:10.1140/epjd/s10053-022-00495-3

EICS:
J. Phys.: Condens. Matter 34 (2022) 374001, DOI: 10.1088/1361-648X/ac7d86

(a)

(b)

Outlook 2023

- **MD simulations of sputtering on different non-planar surfaces (defects,holes, edges …) and their influence on the yields.**
- **Calculating other cross sections (see above), especially excited state cross sections (see above).**
- **More analysis of the Ar/W system, extending it to W+O).**
- **Eurofer sputtering simulations (so far we had problems with Fe potential energy functions)**
- **Combination of BCA and MD at transition from low energies to the BCA limit. First results allow for an optimization of BCA modelling by using MD-derived effective surface binding energies. (Results seem to depend which potential function in BCA is used, not yet understood)**