Computational analysis of physical and chemically assisted physical sputtering in plasma-facing components

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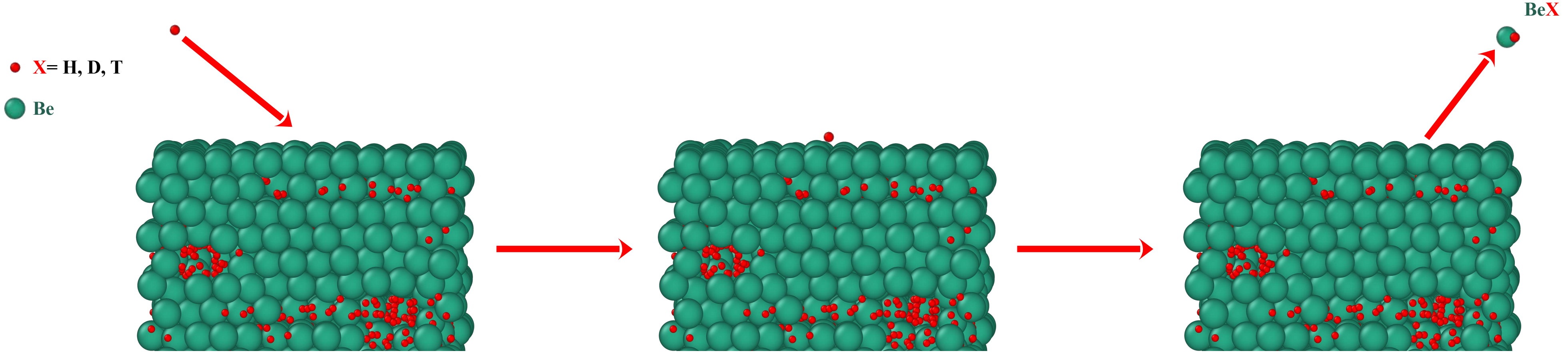
Motivation

- Quantifying erosion and reflection from Beryllium (Be) surfaces, with pre-existing impurity content, using molecular dynamics (MD) simulations
- Evaluating Chemically Assisted Physical Sputtering (**CAPS**) in Be surfaces, for different plasma particle characteristics
- Providing reliable data for Hydrogen (H) and Tritium (T), in addition to Deuterium (D) for further use in ERO2.0 simulations

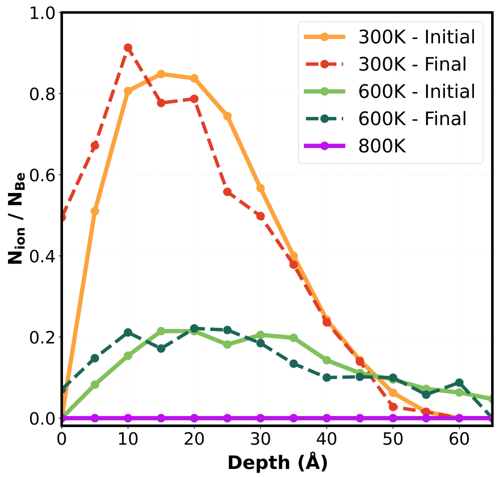


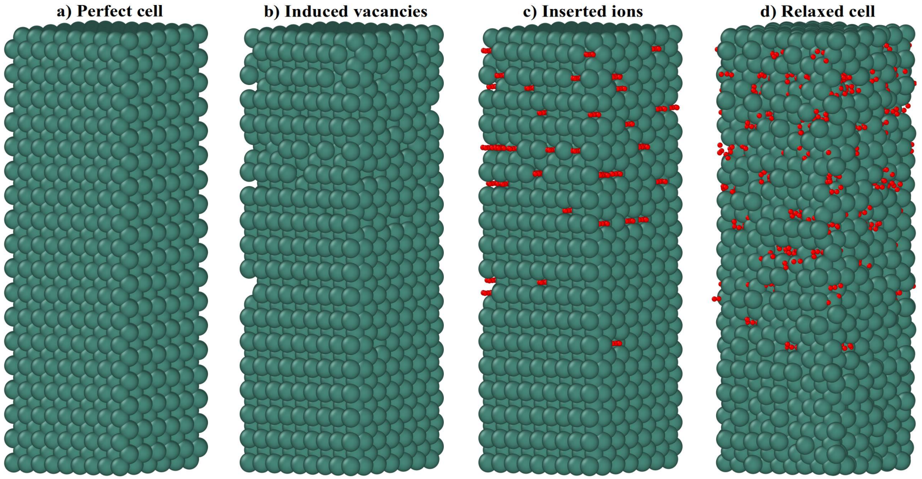
1. Surface Preparation

- **Be** structures were initially loaded with **H/D/T** to set up a pre-existing concentration at different temperatures, based on the density profiles obtained at different surface temperatures through object kinetic Monte Carlo (OKMC) technique [1].

➢ **How?**

- First, 5% of **Be** atoms were removed randomly.
- Then, at each depth range, a certain number of vacancies were selected and 5 ions were inserted in each (based on OKMC and DFT calculations) to obtain the initial distributions.
- Finally, the cells were equilibrated and the final density profiles were obtained.

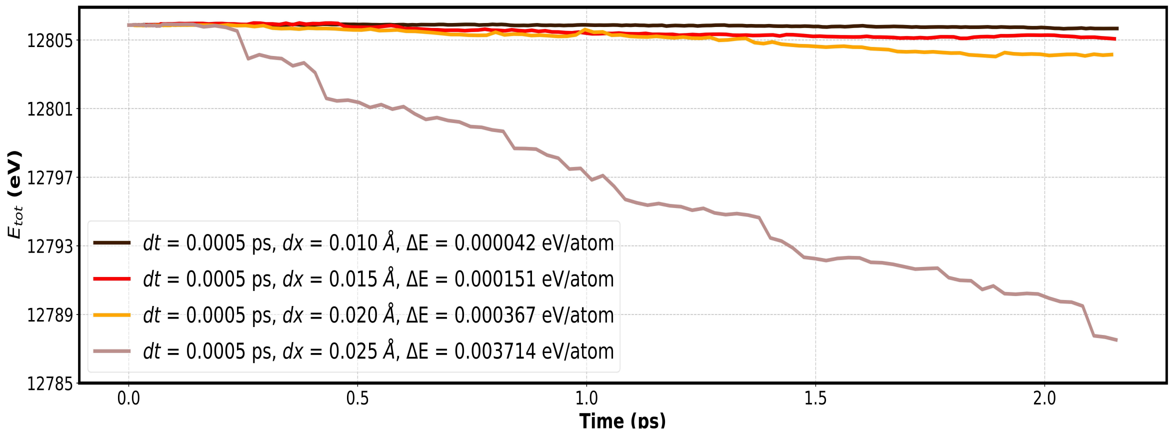


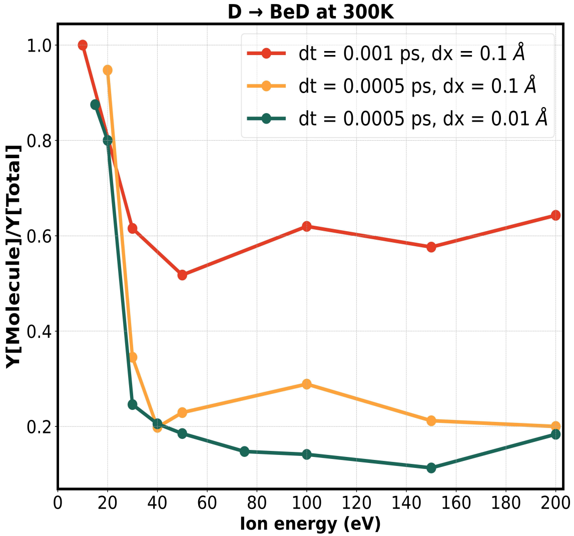


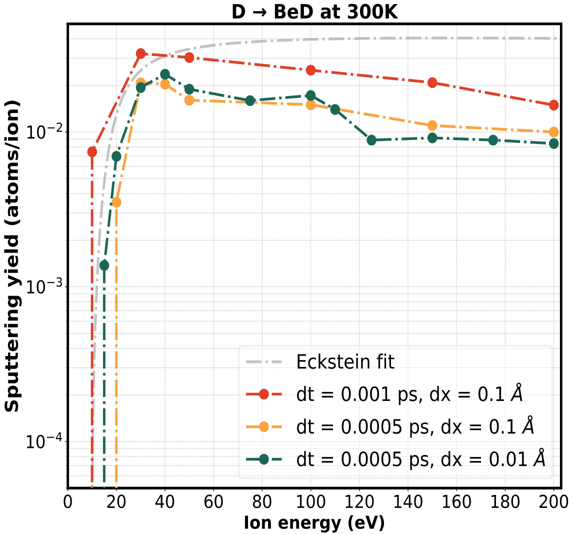
[1] E. Safi et al., Journal of Physics D: Applied Physics (2017).

2. Time step

- Running irradiation simulations with different values for the maximum time step (*dt*) and maximum distance each atom is allowed to move in one step (*dx*).
- Using no thermostat and electronic stopping to prevent any energy dissipation caused by them.
- The best option would be the combination that better preserves the energy of the system.





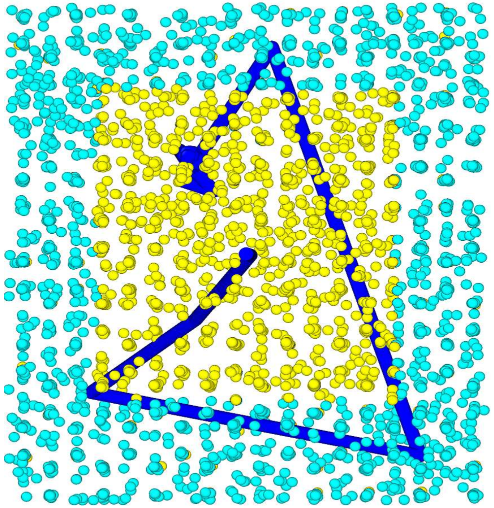


[2] R. Behrisch and W. Eckstein, Springer (2007).

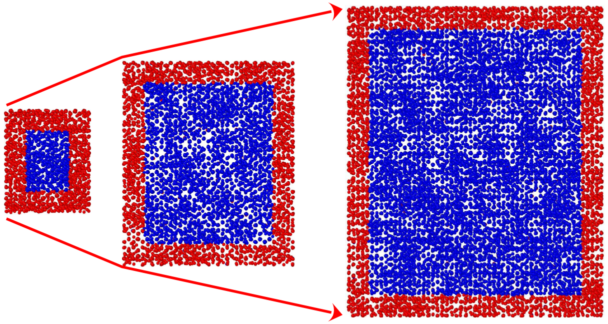
3. Cell Size

- To minimize the interaction between the incident ion and the boundary region, 3 different cell sizes were prepared and used for different impact energies and angles.

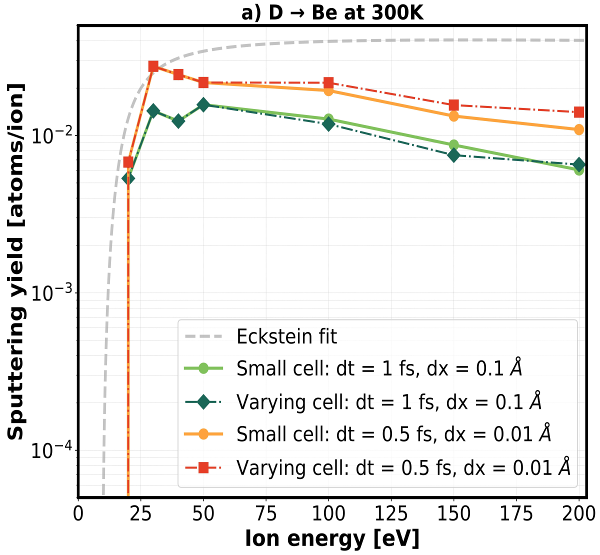
Plasma particle going in the boundary region



Increasing the cell size by replicating in X and Y directions



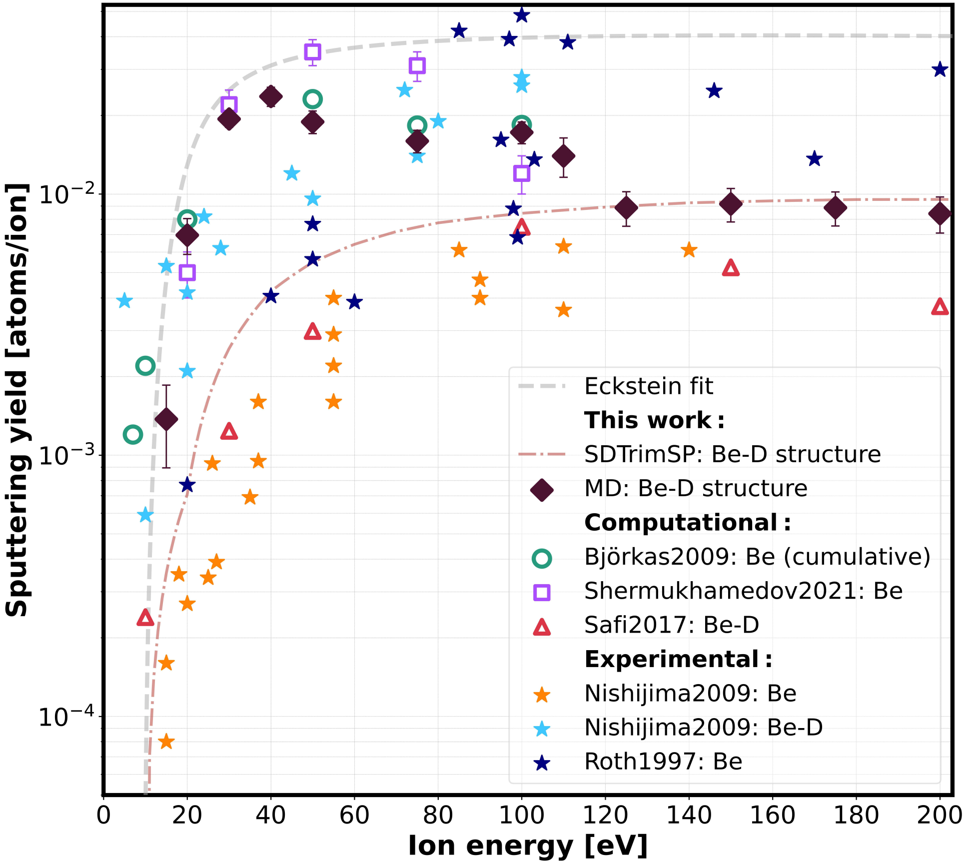
Effect of cell size on sputtering yield



[2] R. Behrisch and W. Eckstein, Springer (2007).

Sputtering Yield

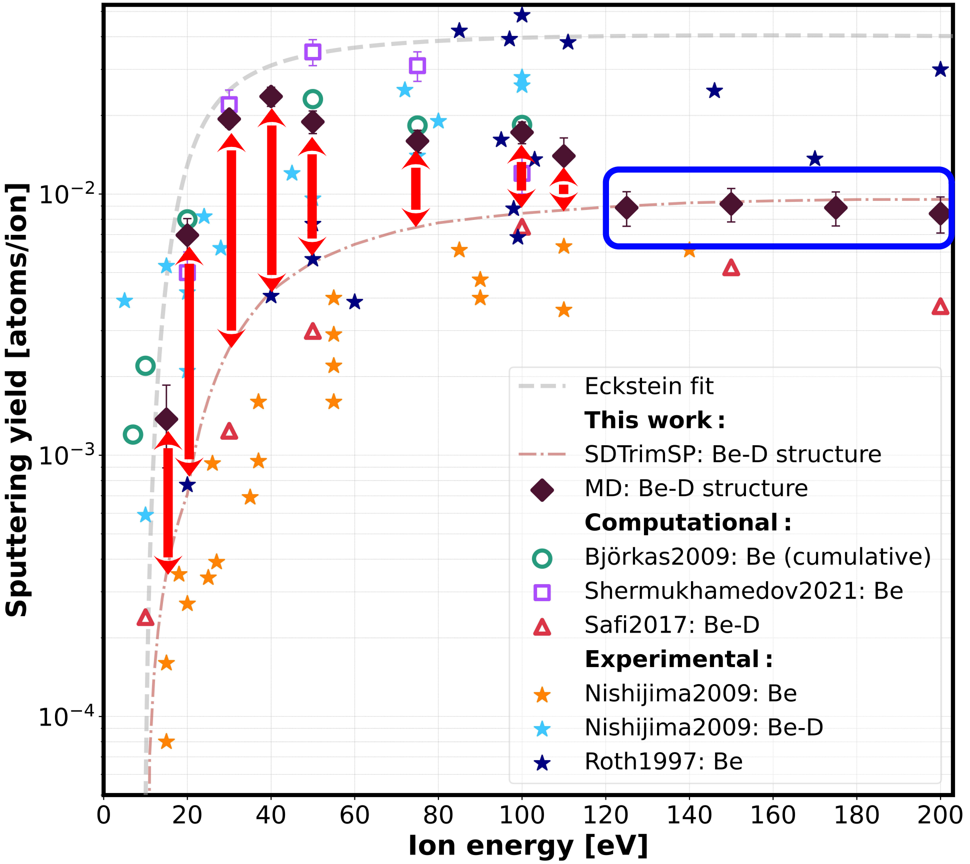
- The figure represents the total sputtering yield of Be-D structure at 300K for normal incidence.
- Good agreement with the experimental values for Be with D present in the structure (light blue stars)
- Overall, no decreasing trend in the yield for impact energies higher than 50 eV



[1] E. Safi et al., Journal of Physics D: Applied Physics (2017).
[2] R. Behrisch and W. Eckstein, Springer (2007).
[3] C. Björkas et al., New Journal of Physics (2009).
[4] S. Shermukhamedov et al., Nuclear Fusion (2021).
[5] D. Nishijima et al., Journal of Nuclear Materials (2009).

Sputtering Yield

- Large difference between MD and SDTrimSP yields at low energies is observed.
- The agreement at high energies is very good.
- This emphasizes on the importance of CAPS at low energies.

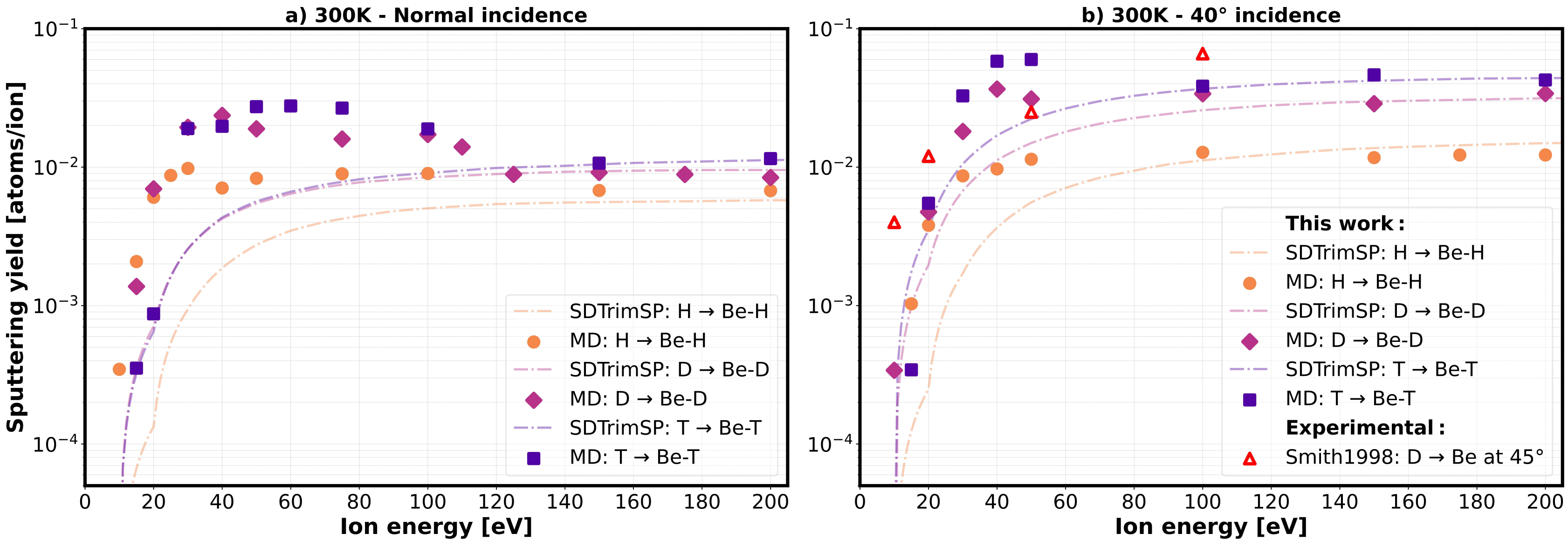


[1] E. Safi et al., Journal of Physics D: Applied Physics (2017).
[2] R. Behrisch and W. Eckstein, Springer (2007).
[3] C. Björkas et al., New Journal of Physics (2009).
[4] S. Shermukhamedov et al., Nuclear Fusion (2021).
[5] D. Nishijima et al., Journal of Nuclear Materials (2009).

Sputtering Yield

H isotope

- In general, increasing the isotope mass will result in an increase in the sputtering yield due to a more efficient momentum transfer.
- Good agreement is observed with SDTrimSP results for all isotopes at higher impact energies.

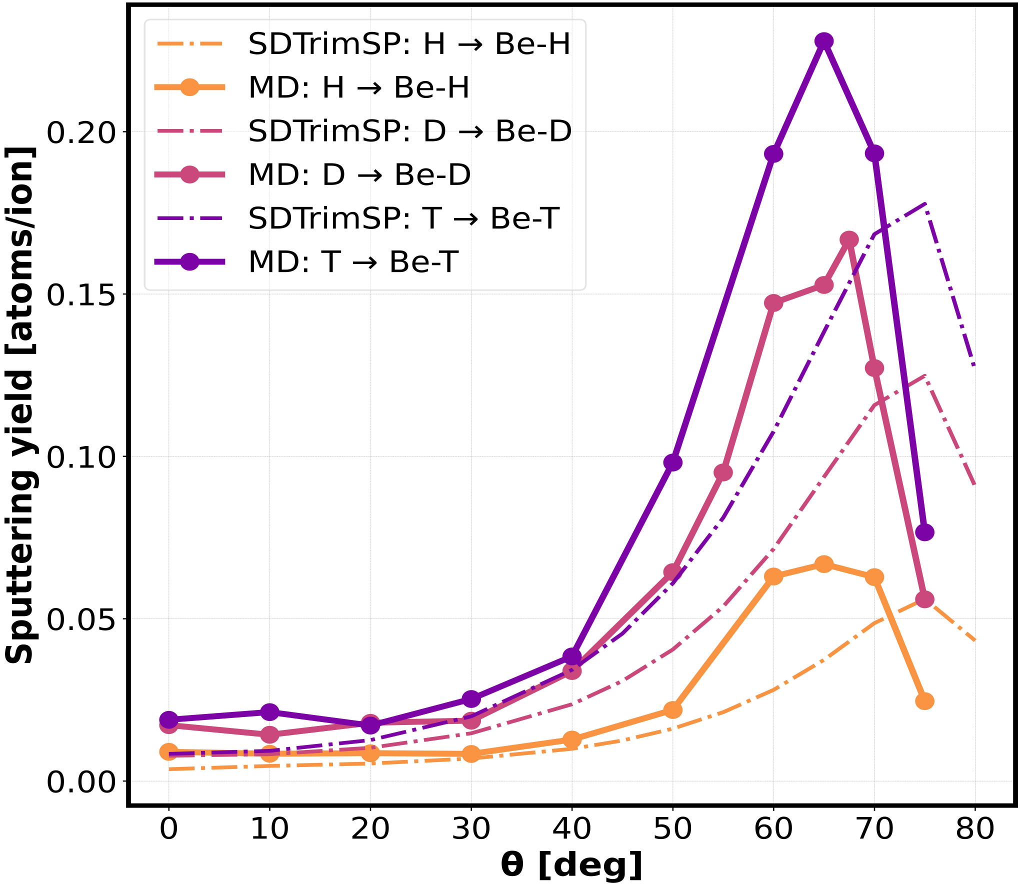


[6] P.C. Smith and D.N. Ruzic, Nuclear Fusion (1998).

Sputtering Yield

Impact angle

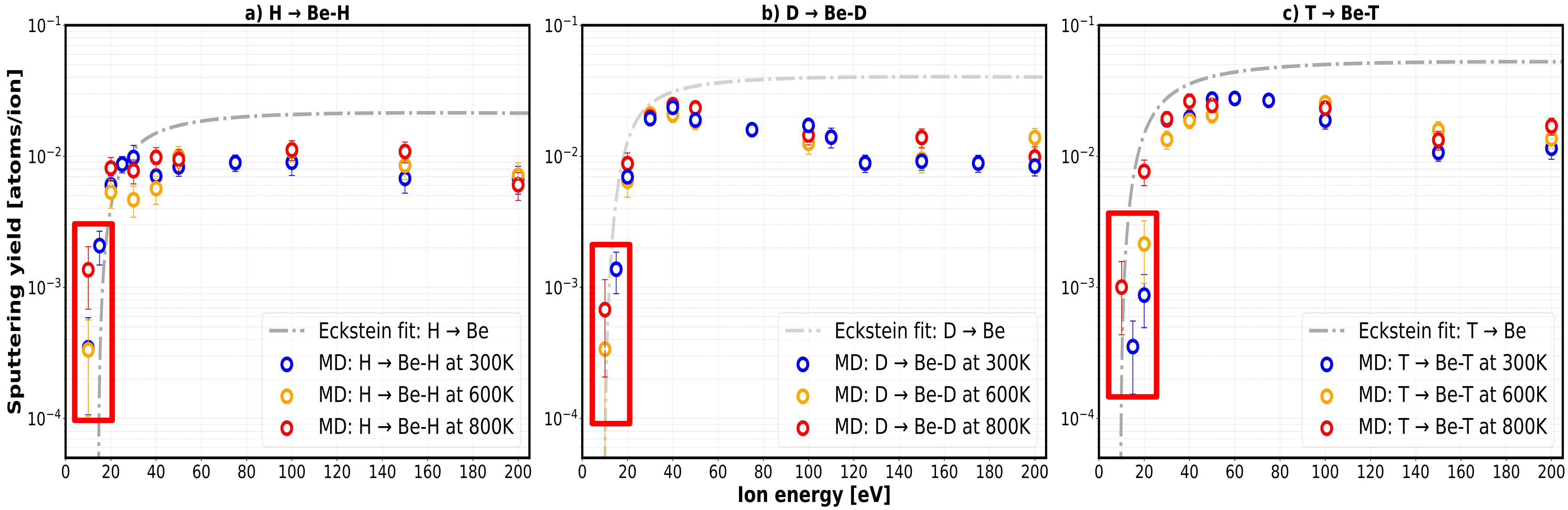
- Increasing the impact angle from 0° to ~ 65° increases the sputtering yield.
- Further increments will result in a sharp decrease of the sputtering yield.
- Same behavior is observed for all isotopes, with only difference being the magnitude of the yield.
- Compared to SDTrimSP data we get higher yield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



➢ Sputtering Yield

• Surface temperature

➢ In general, a lower sputtering threshold is observed at higher surface temperatures.

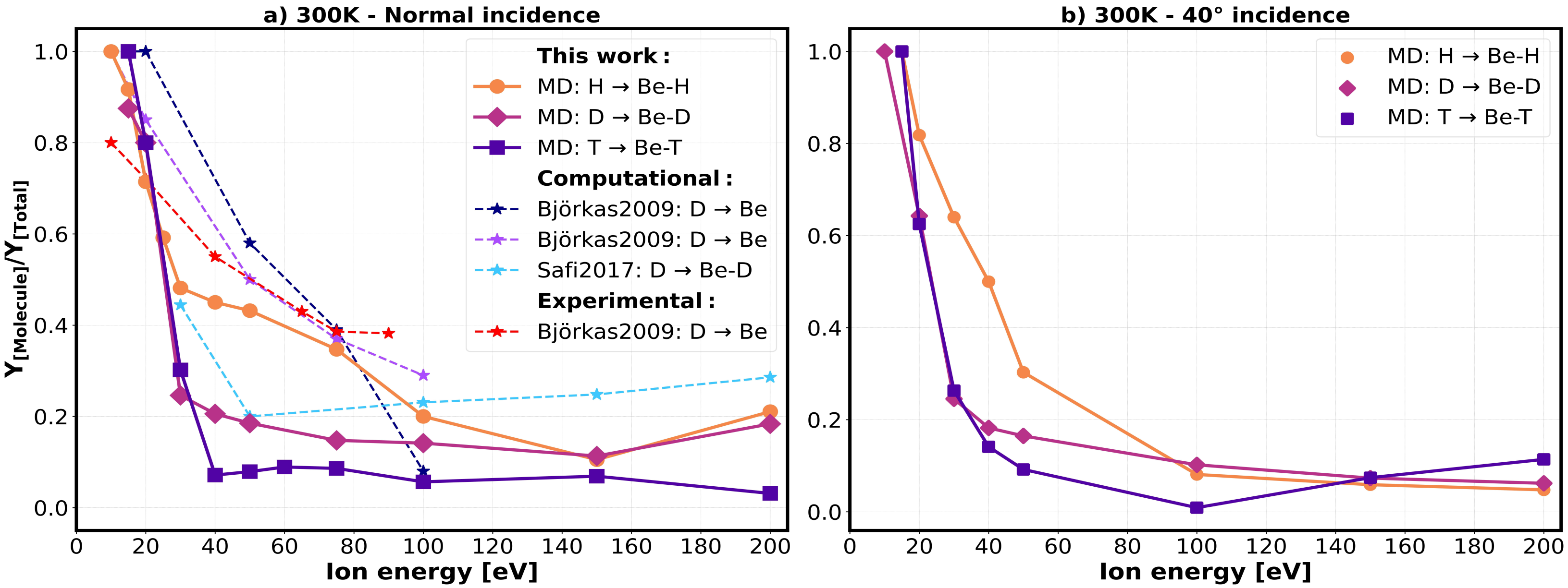


[2] R. Behrisch and W. Eckstein, Springer (2007).

CAPS

Impact energy

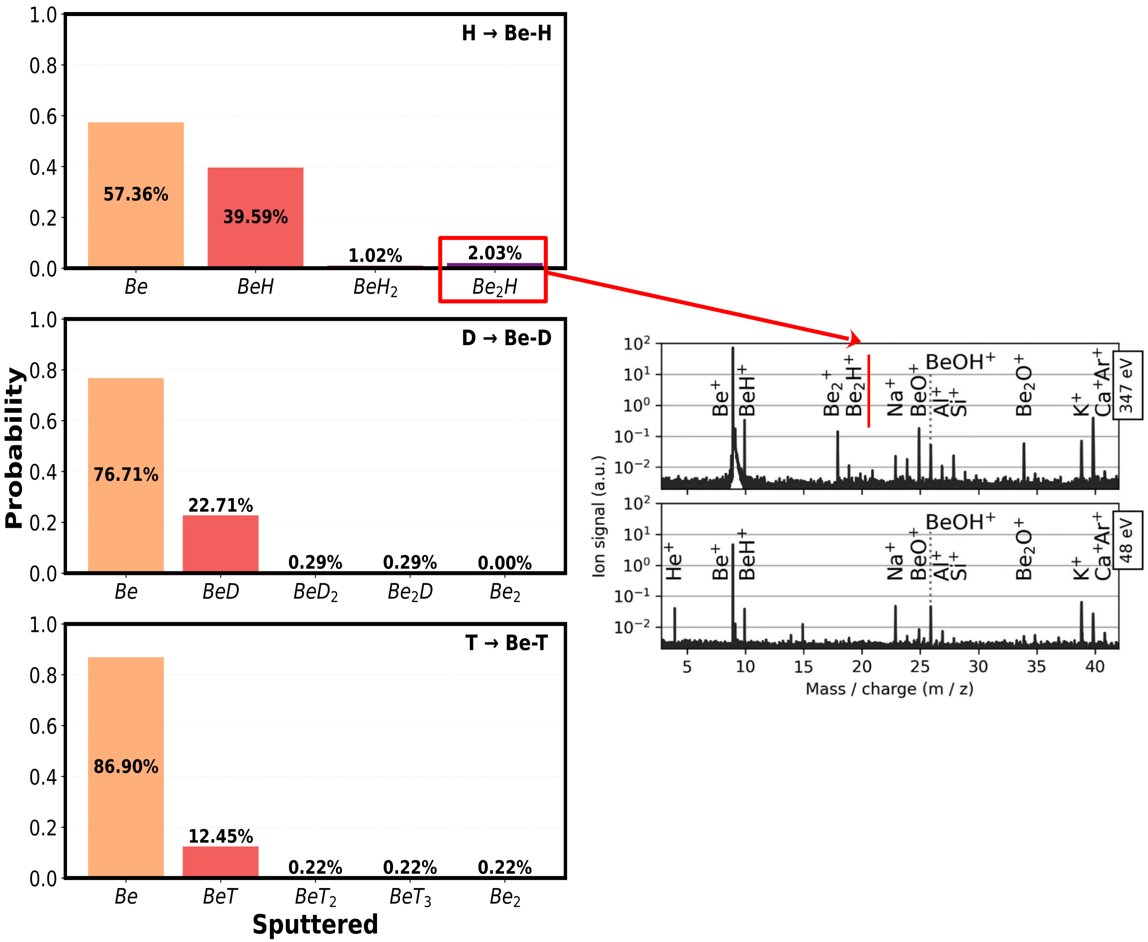
- The higher the impact energy, the lower the probability of CAPS will be.
- Same trend has been observed for all isotopes.



[1] E. Safi et al., Journal of Physics D: Applied Physics (2017).
[3] C. Björkas et al., New Journal of Physics (2009).

CAPS

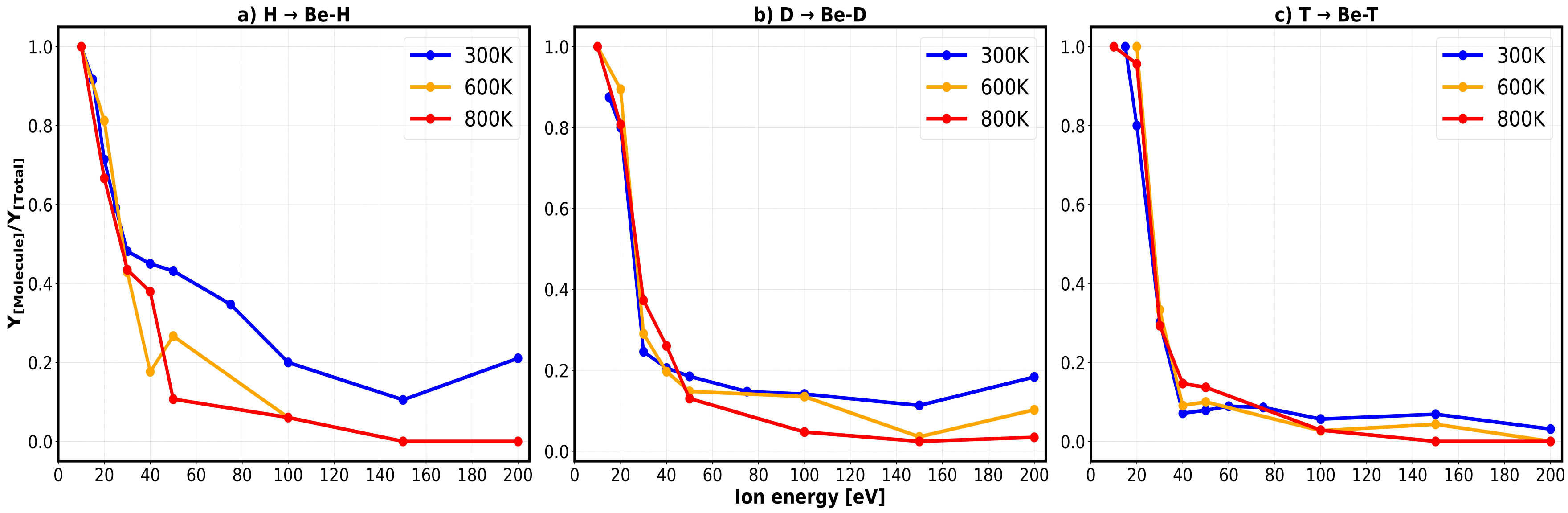
- **H isotope**
  - Moving from the lightest (H) to the heaviest isotope (T) the probability of CAPS decreases strongly.
  - This could be resulted from a longer interaction time between H and Be and a less momentum transfer due to a larger mass difference.



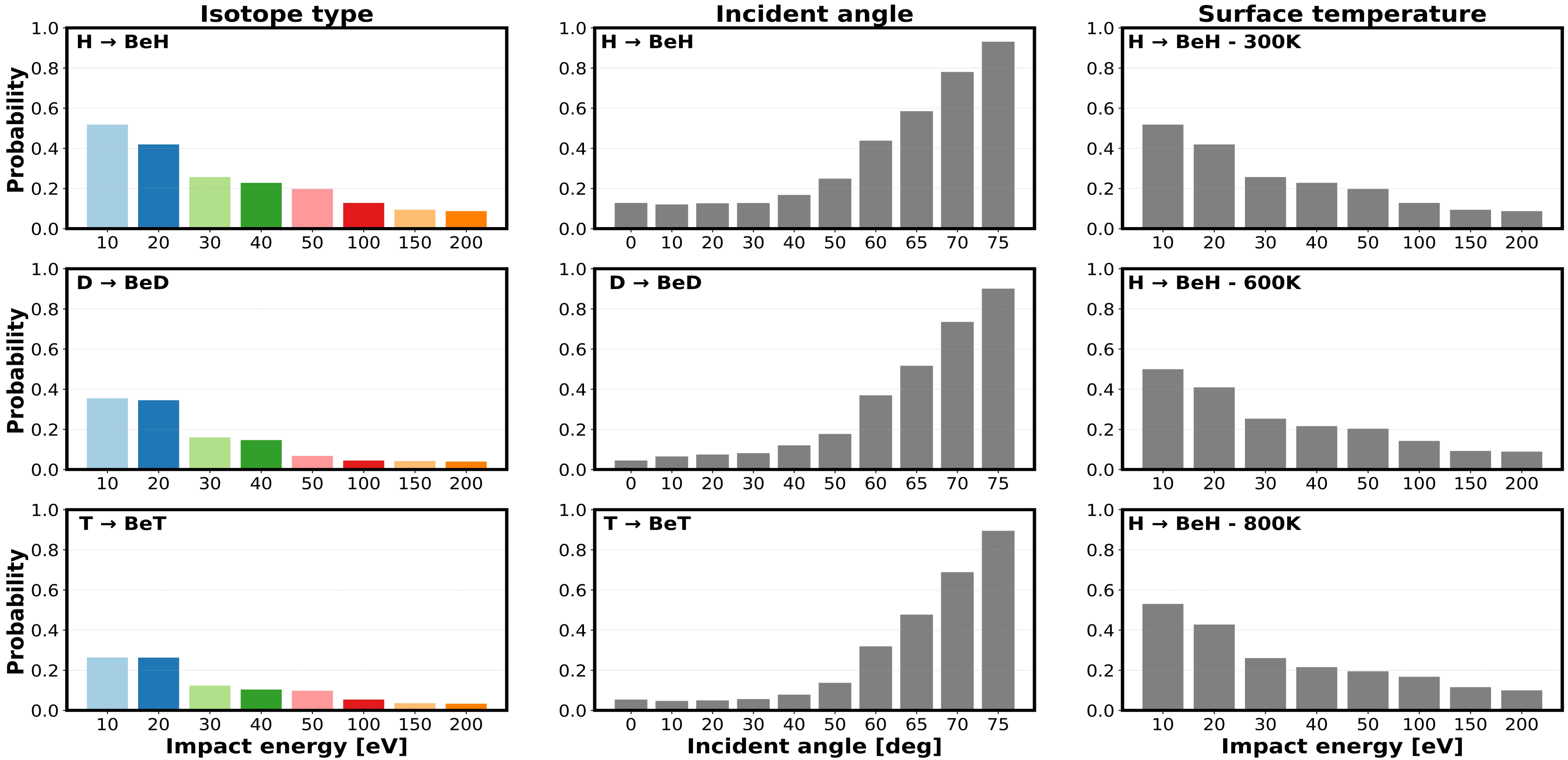
[7] F. Duensing et al., Nuclear Materials and Energy (2022).

CAPS

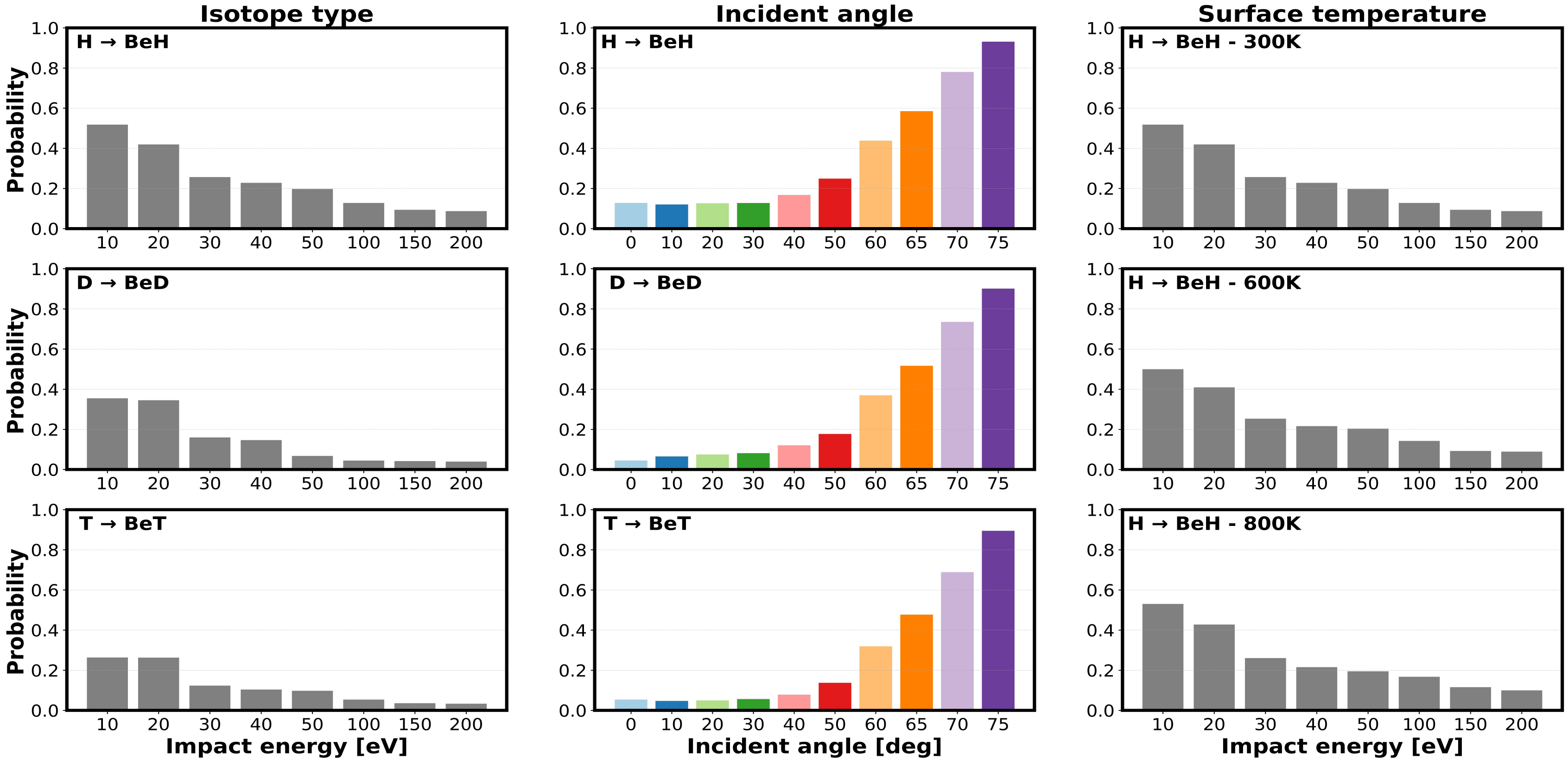
- **Surface temperature**
  - **H:** lower CAPS contribution at elevated surface temperatures.
  - **D/T:** increased CAPS contribution at low energies and decreased contribution at high energies.



Reflection

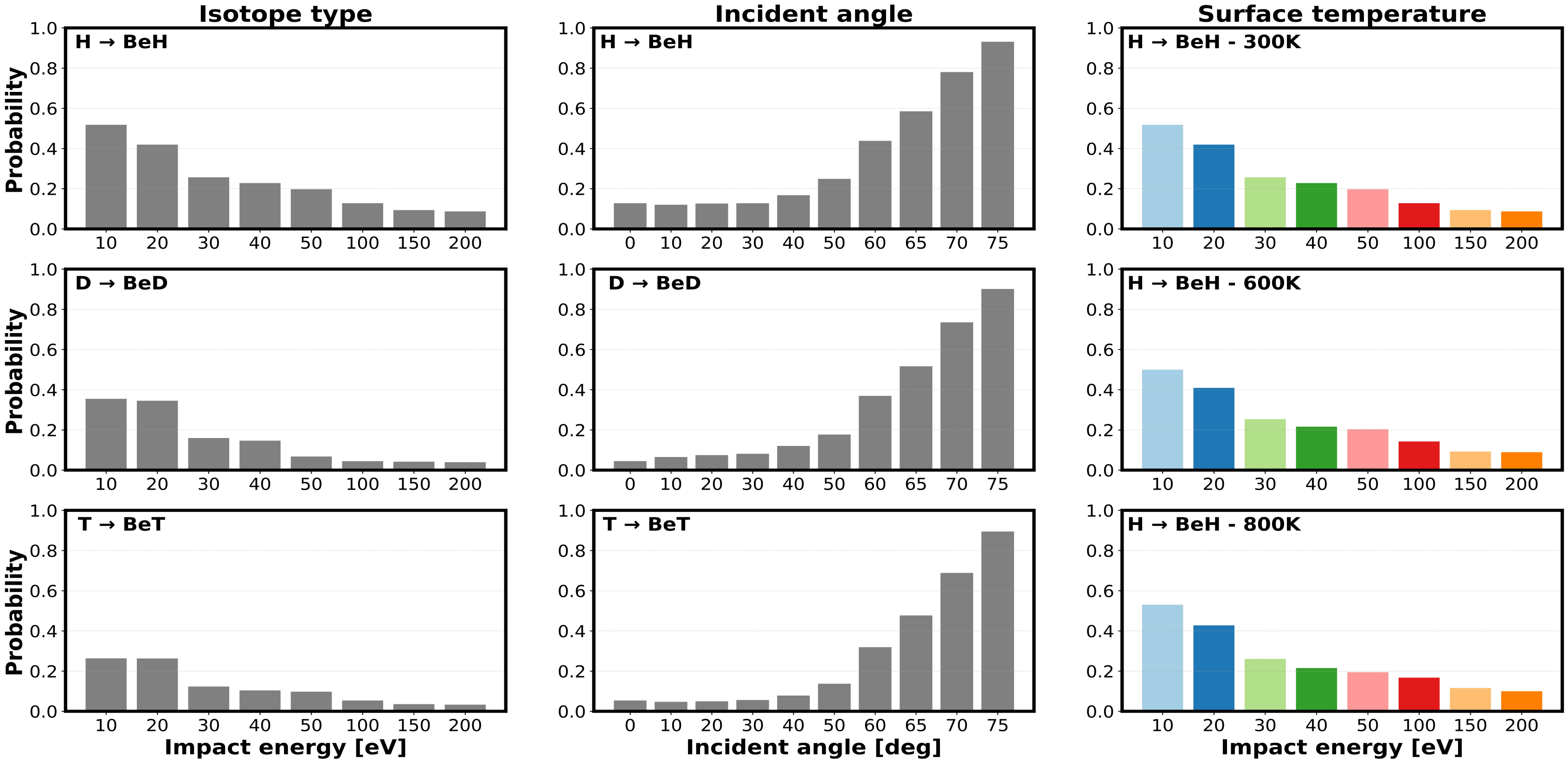

Isotope type
Incident angle
Surface temperature
H → BeH
D → BeD
T → BeT
H → BeH - 300K
H → BeH - 600K
H → BeH - 800K
Probability
Impact energy [eV]
Incident angle [deg]

Reflection



Isotope type
Incident angle
Surface temperature
H → BeH
D → BeD
T → BeT
H → BeH - 300K
H → BeH - 600K
H → BeH - 800K
Probability
Impact energy [eV]
Incident angle [deg]

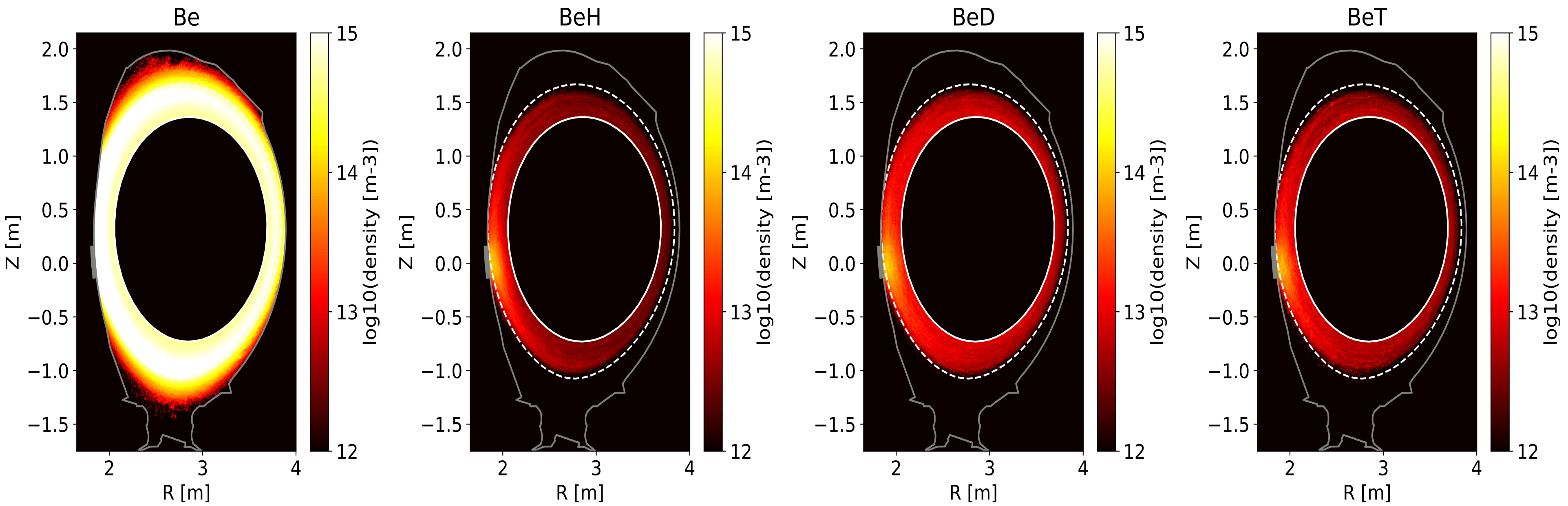
Reflection



Isotope type
Incident angle
Surface temperature
H → BeH
D → BeD
T → BeT
H → BeH - 300K
H → BeH - 600K
H → BeH - 800K
Probability
1.0
0.8
0.6
0.4
0.2
0.0
10
20
30
40
50
100
150
200
0
60
65
70
75
Impact energy [eV]
Incident angle [deg]

➢ ERO2.0

- The MD data have been implemented in ERO2.0 and tests are being performed to benchmark the results.



- The size of the cells and the time step significantly influence the simulations and must be chosen with care.

- Findings show a significant reliance of the sputtering yield, CAPS, and reflection on the characteristics of the plasma particle.

- MD results are in strong agreement with SDTrimSP results for sputtering yield at high impact energies.

- Nonetheless, inability of SDTrimSP to incorporate CAPS highlights the essential role of MD, especially at lower energy levels.

Thanks for your attention!

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