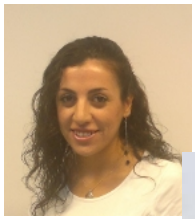
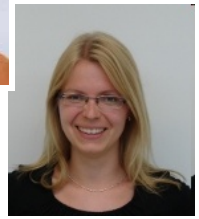
Combined molecular dynamics and kinetic Monte Carlo modelling to simulate D deposition and Be sputtering at realistic fluxes.

Elnaz Safi,

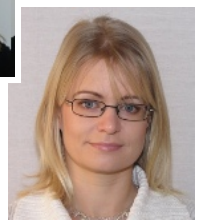


Ane Lasa,

Carolina Björkas,



Andrea Sand,



and Kai Nordlund

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Fusion reactor mat'ls

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Dr. Andrey Ilinov
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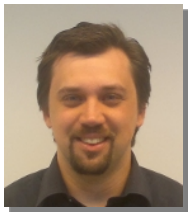
M Sc Laura Bukonte
Fusion reactor mat'ls



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Dr Ville Jansson
Particle physics mat'ls

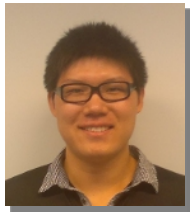
Dr Andreas Kyritsakis
Particle physics mat'ls

M Sc Wei Ren
Carbon nanostructures

M Sc Fredric Granberg
Dislocations

M Sc Morten Nagel
Nuclear materials

M Sc Elnaz Safi
Fusion reactor mat'ls



M Sc Junlei Zhao
Nanoclusters

M Sc Anders Korsbäck
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M Sc Ekaterina Baibuz
Particle physics mat'ls

M Sc Mihkel Veske
Particle physics mat'ls

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Surface ripples

M Sc Shuo Zhang
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Mr Jesper Byggmästar
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M Sc Simon Vigonski
Particle physics mat'ls

M Sc Henrique Muinoz
Swift heavy ions

Mr Christoffer Fridlund
Ion beam processing

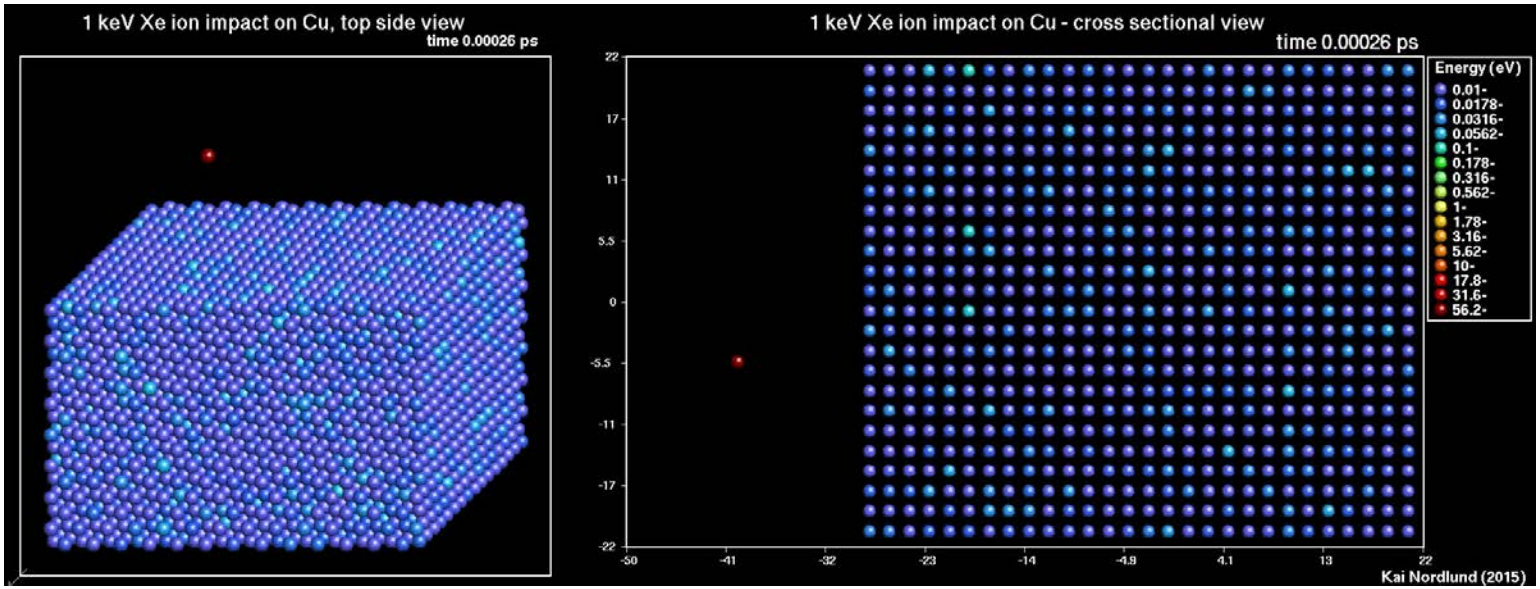
Ms Jonna Romppainen
Atom probe tomography

Contents

- **Reminders of background:**
  - Molecular dynamics
  - The rich materials science of plasma-wall interactions
  - Swift chemical sputtering of Be
- **Results for H isotope interactions with Be by combined MD and KMC modelling**

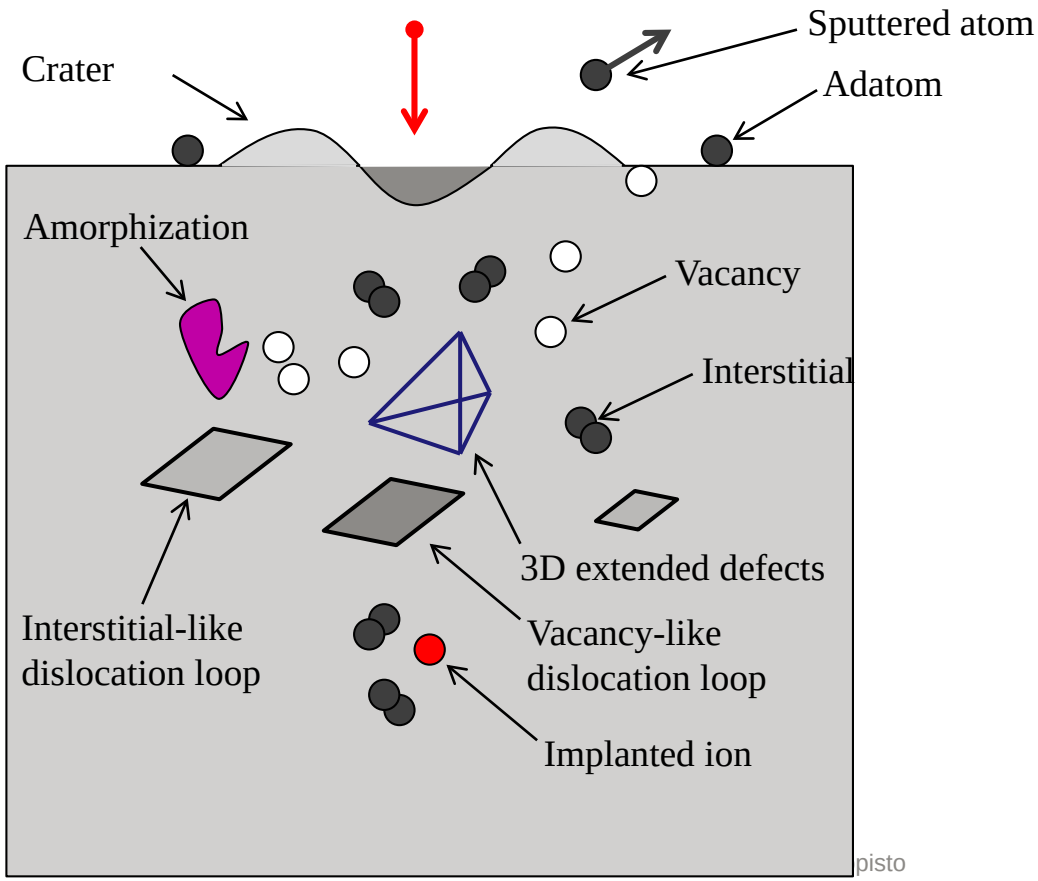
MD simulations of radiation effects

- Molecular dynamics simulations: solving Newton's equations of motion of a system of atoms
- A basic MD code can be written in 2 days and is < 1000 code lines, a modern parallel one > 5 person-years and > 10 0000 lines of code
- Basic simple example:



The rich materials science of plasma-wall interactions

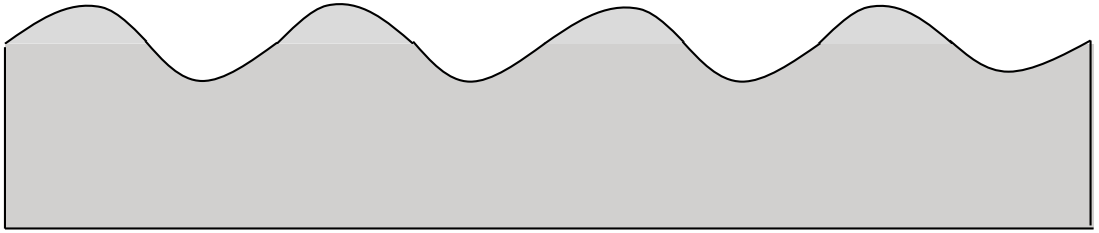
Just for a single ion all of the below effects *may* be produced:



The rich materials science of plasma-wall interactions: high fluences

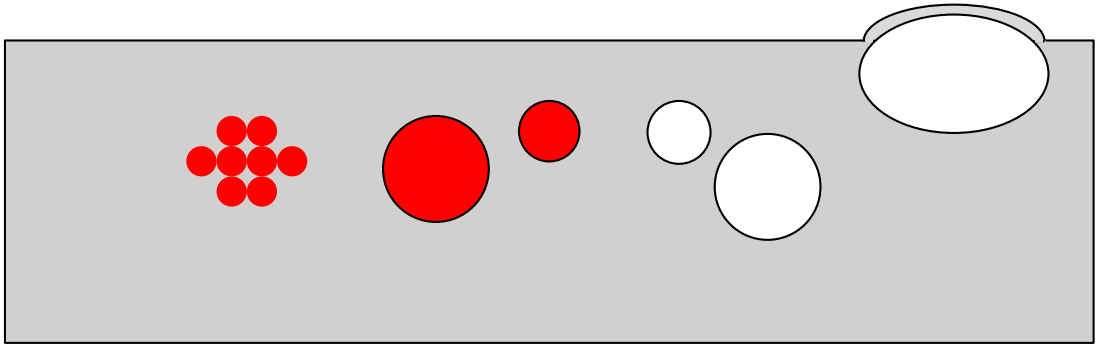
In addition, for multiple ions i.e. prolonged irradiation many more things can happen, for instance:

Spontaneous roughening/ripple formation



[T. K. Chini, F. Okuyama, M. Tanemura, and **K. Nordlund,** Phys. Rev. B **67**, 205403 (2003); Norris et al, Nature communications **2**, 276 (2011)]

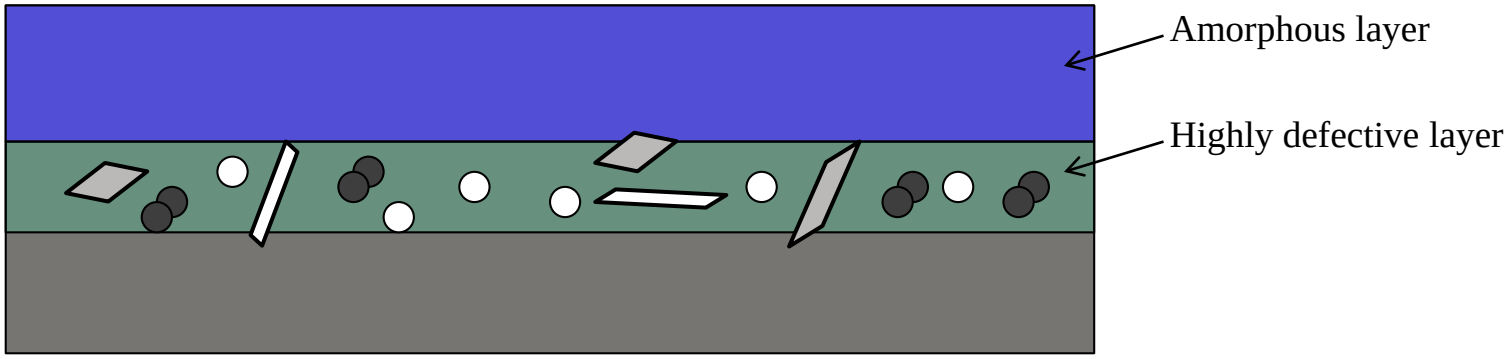
Precipitate/nanocluster, bubble, void or blister formation inside solid



[Bubbles e.g: K. O. E. Henriksson, **K. Nordlund**, J. Keinonen, D, Physica Scripta **T108**, 95 (2004); Nanocrystals e.g. 75S. Dhara, Crit. Rev. Solid State Mater. Sci. 32, 1 [2007)]

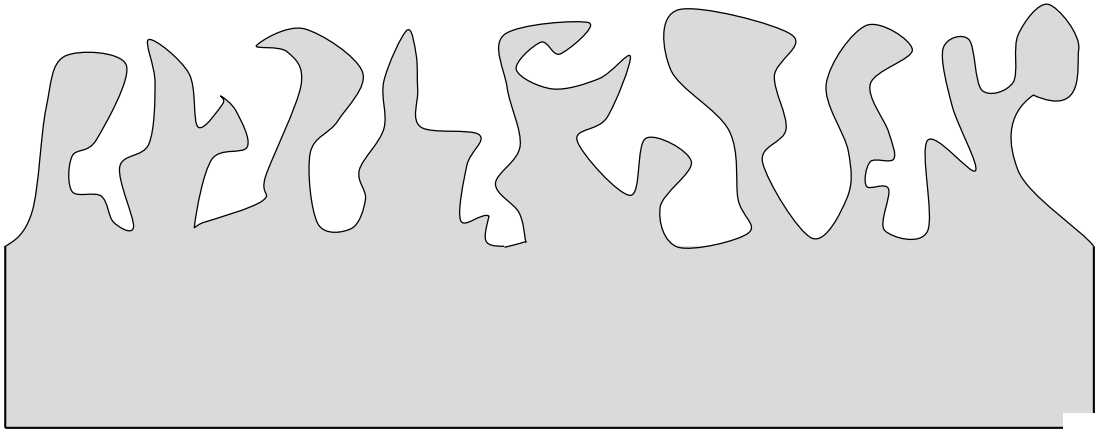
The rich materials science of plasma-wall interactions: high fluences

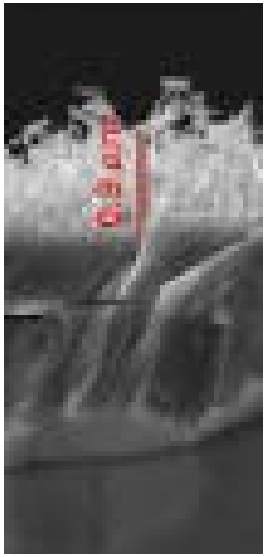
Phase changes, e.g. amorphization:



Spontaneous porousness formation, “fuzz”

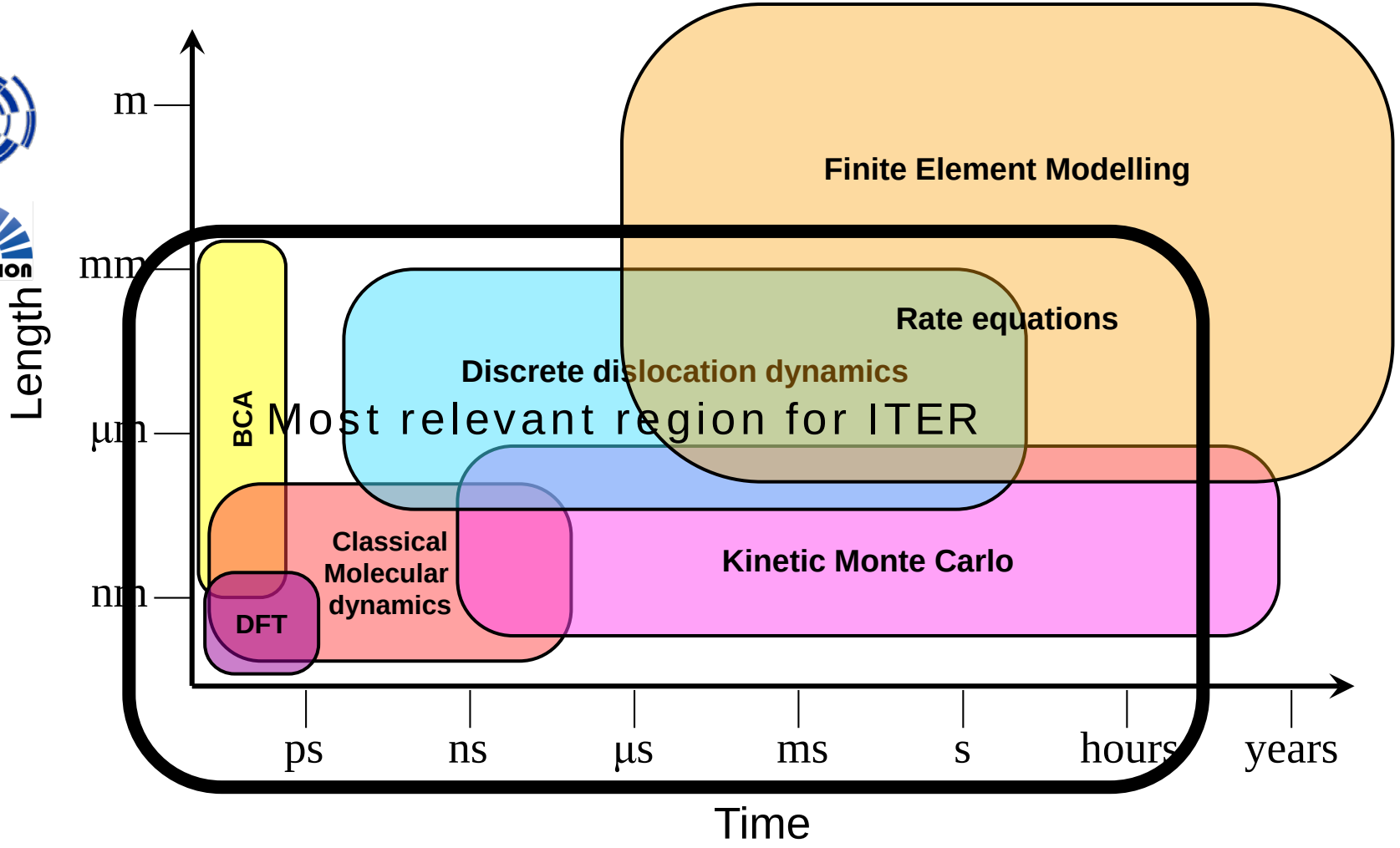
Highly fusion-relevant now, He -> W does it





[http://vlt.ornl.gov/research/20110119_highlight_doerner.pdf]

Simulation framework to handle all this



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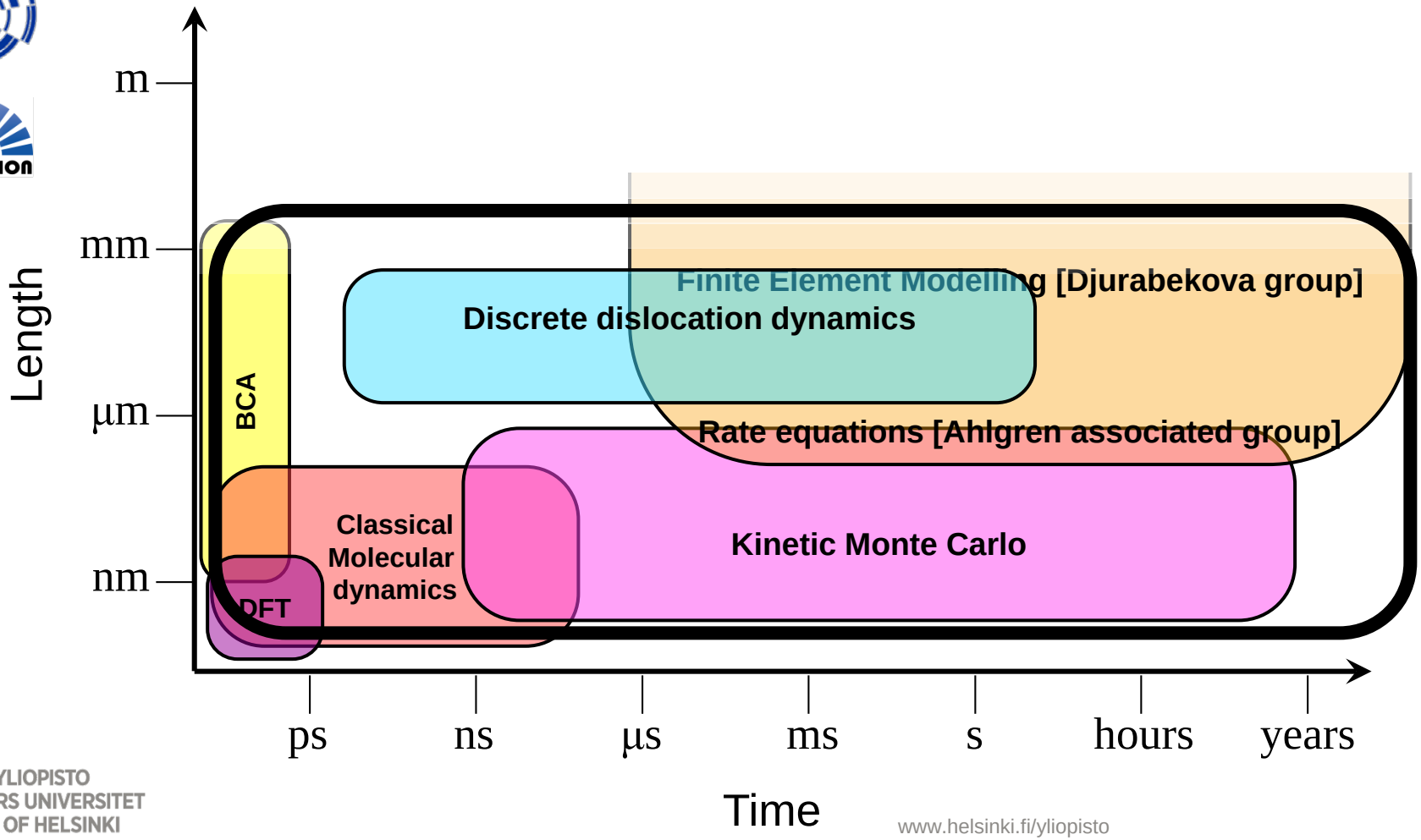
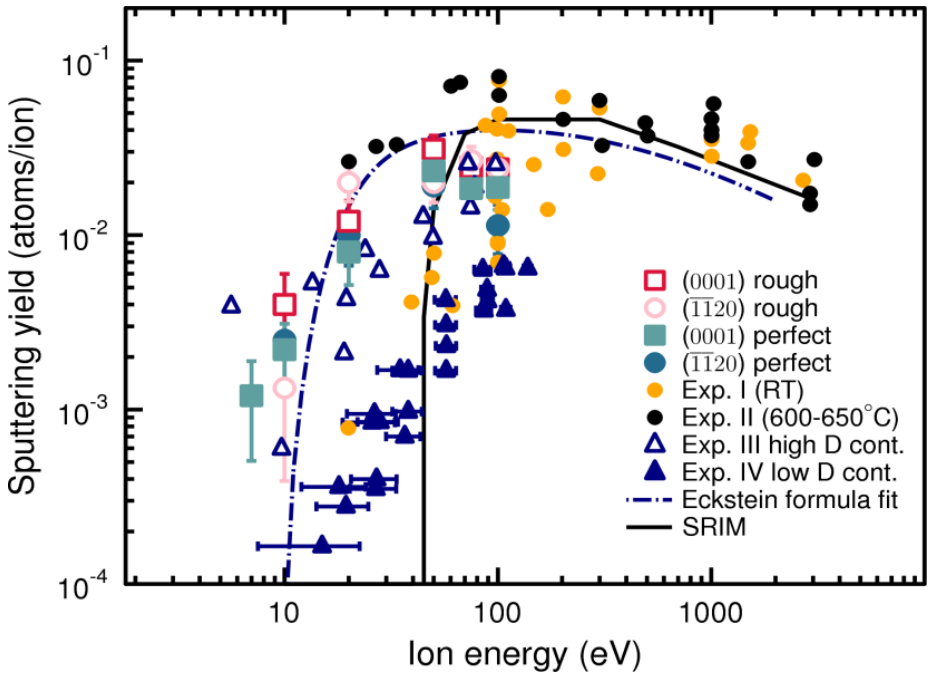
[For a review see: K. Nordlund, C. Björkas, T. Ahlgren, , A. Lasa, and A. E. Sand, *Multiscale modelling of plasma-wall interactions in fusion reactor conditions*, J. Phys. D: Appl. Phys. **47**, 224018 (2014), Invited paper for Special Issue on Fundamentals of plasma-surface interactions].

Range of work in our groups



Old results: Sputtering of initially pure Be by D

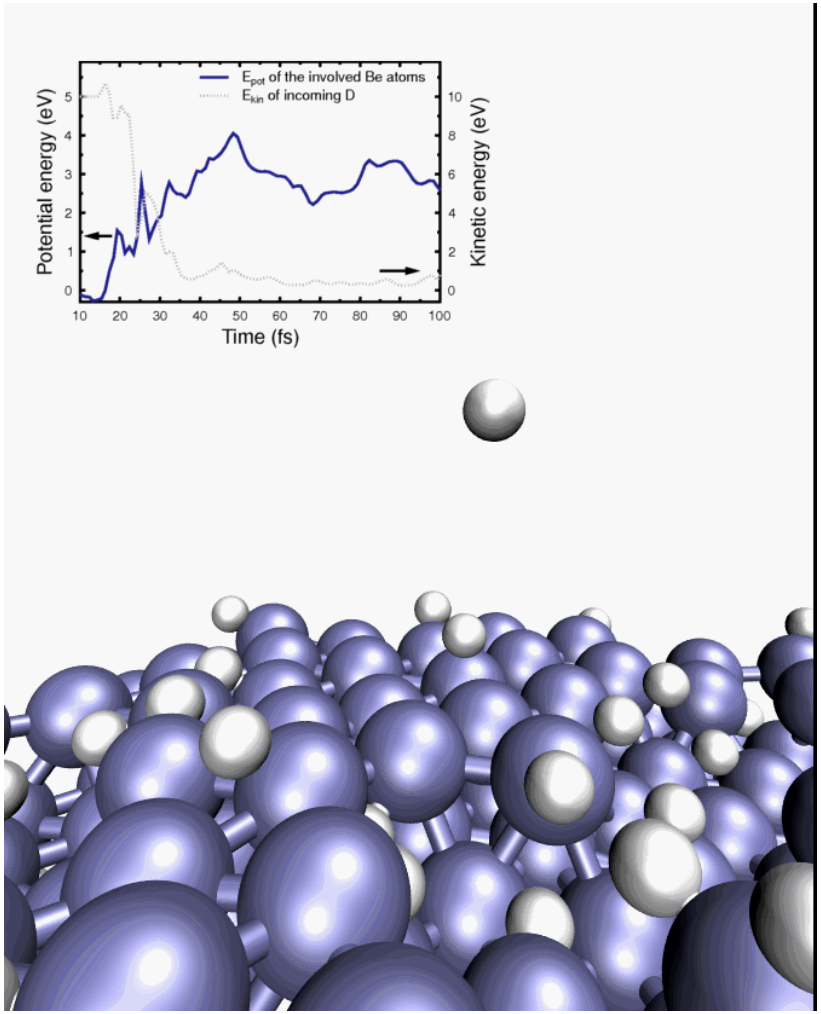
- Our simulations agree with plasma experiments done at the PISCES-B facility at low energies
  - At higher energies with the rest
- Sputtering is seen at 7 eV!



[C. Björkas, K. Vörtler, K. Nordlund, D. Nishijima, and R. Doerner, New J. Phys. 11, 123017 (2009)]

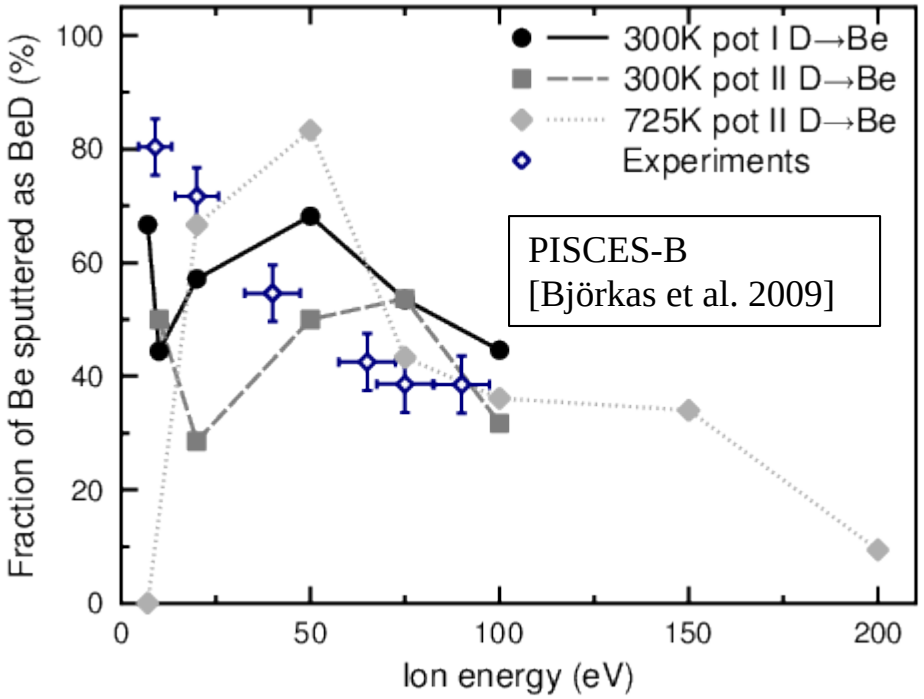
Old results:
Sputtering of initially pure Be by D

- The low-E sputtering is explained by swift chemical sputtering



D irradiation of initially pure Be

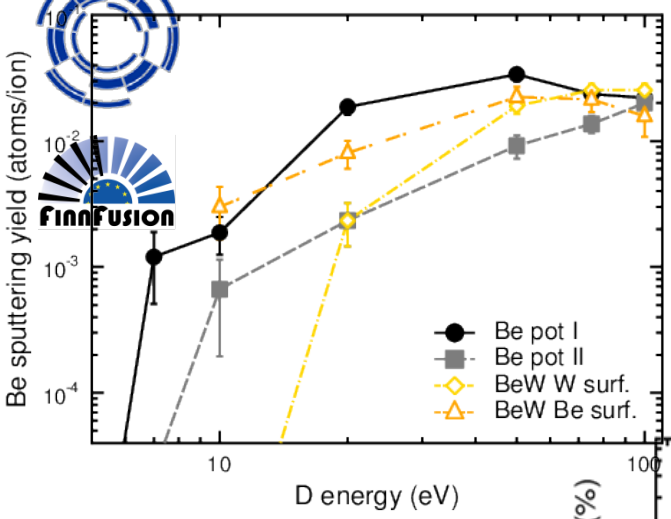
- At low energies a large fraction of Be is eroded as BeD molecules
  - **Chemical sputtering!**
- This fraction decreases with ion energy
- This collaboration came out of a previous IAEA meeting with Doerner!

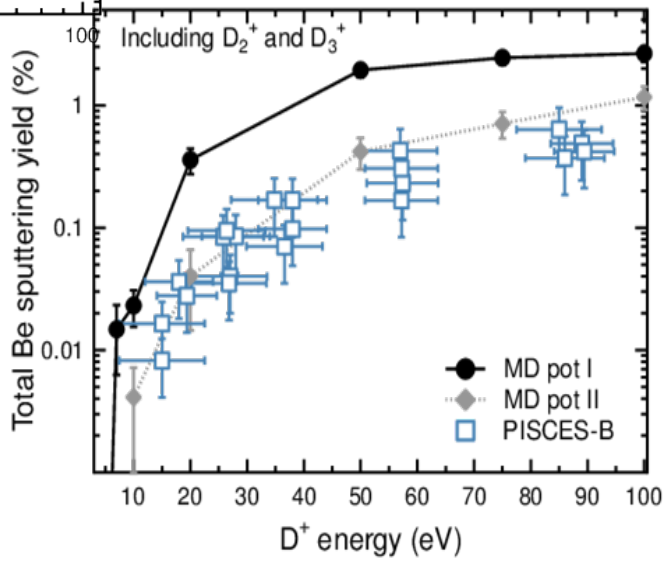


Old results on Be sputtering

Potential dependence

The sputtering yield of pure Be depends on the potential





Pot I vs Pot II:
Pot I has:

- Larger cutoff
- Different elastic constants
- Different thermal expansion
- **Lower surface binding energy**

[C. Björkas et al, Plasma Physics and Controlled Fusion **55**, 074004 (2012)]

Limitations of old work

- Time scale of MD: flux is very high → no time for D migration → H surface concentration may be too high

- Apparent dilemma: experiments do not observe any (or very little) BeD_2 , while these simulations show a lot
- **Possible solution 1**: DFT calculations from Michael Probst's group indicate the BeD_2 is fairly unstable and will in a plasma likely decay quickly into Be + D_2 or BeD + D
- **Possible solution 2**: too little D migration overestimates D surface concentration?

Motivation for current work

- We wanted to understand the relationship between Be surface temperature, D concentration and sputtering yields for plasma-surface interaction (PSI) studies:

Be erosion:

a) Need for modeling to provide detail description on the underlying mechanism

b) **MD** modeling of Be exposed to D: a parameter scan

Parameters known to affect erosion:

- Energy (E_{imp})
- Angle (α_{imp})

} Commonly studied

- Flux (Γ_{imp})
- Surface temperature (T_{surf})
- Deuterium concentration (c_D)

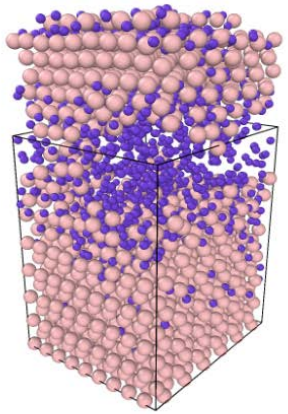
} Little known

Motivation

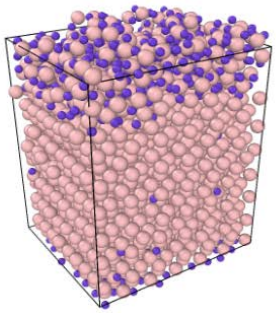
MD modeling of D → Be: T_{surf} and c_D

- T_{surf}: cumulative D impacts on Be show a complex outcome for molecular erosion
  - Larger molecules are also emitted when c_D increases on the topmost layer
  - Due to very different D profiles:

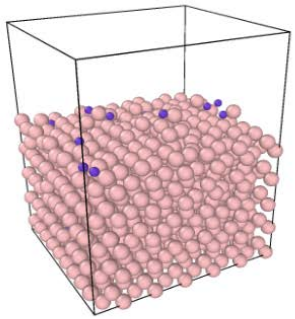
$T_{surf} \sim$
- < 600K → D implantation
- 600-900K → D at topmost layers
- > 900K → D_2 desorption



(a): T = 200 K



(b): T = 600 K



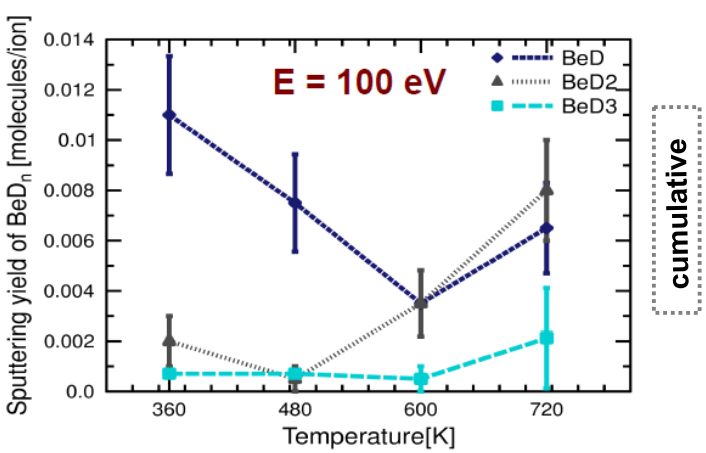
(c): T = 1440 K

E. Safi et al., JNM 463 (2014)

Motivation

Complex relationship T_{surf}- c_D

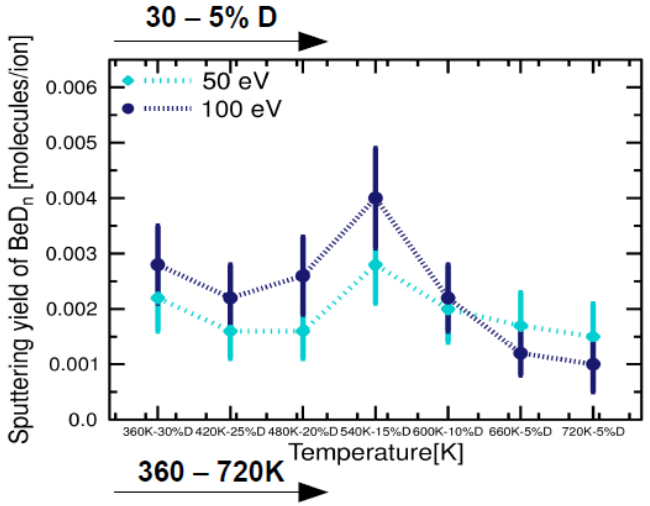
- There is a complex relationship between T_{surf} and c_D
- Non-cumulative simulations to study T_{surf} and c_D independently
- c_D from cumulative irradiation cannot be assumed "in equilibrium" → Estimate (based on indirect experimental deductions by S. Brezinsek) c_D = 30% for low T_{surf}~ 360K and c_D = 5% for high T_{surf}~ 800K



cumulative

E. Safi et al., JNM 463 (2014)

non-cumulative



- The outcome soon diverged from JET observations

=> A rigorous study of $c_D = c_D(T_{surf})$ needed

A true multiscale approach: MD + KMC

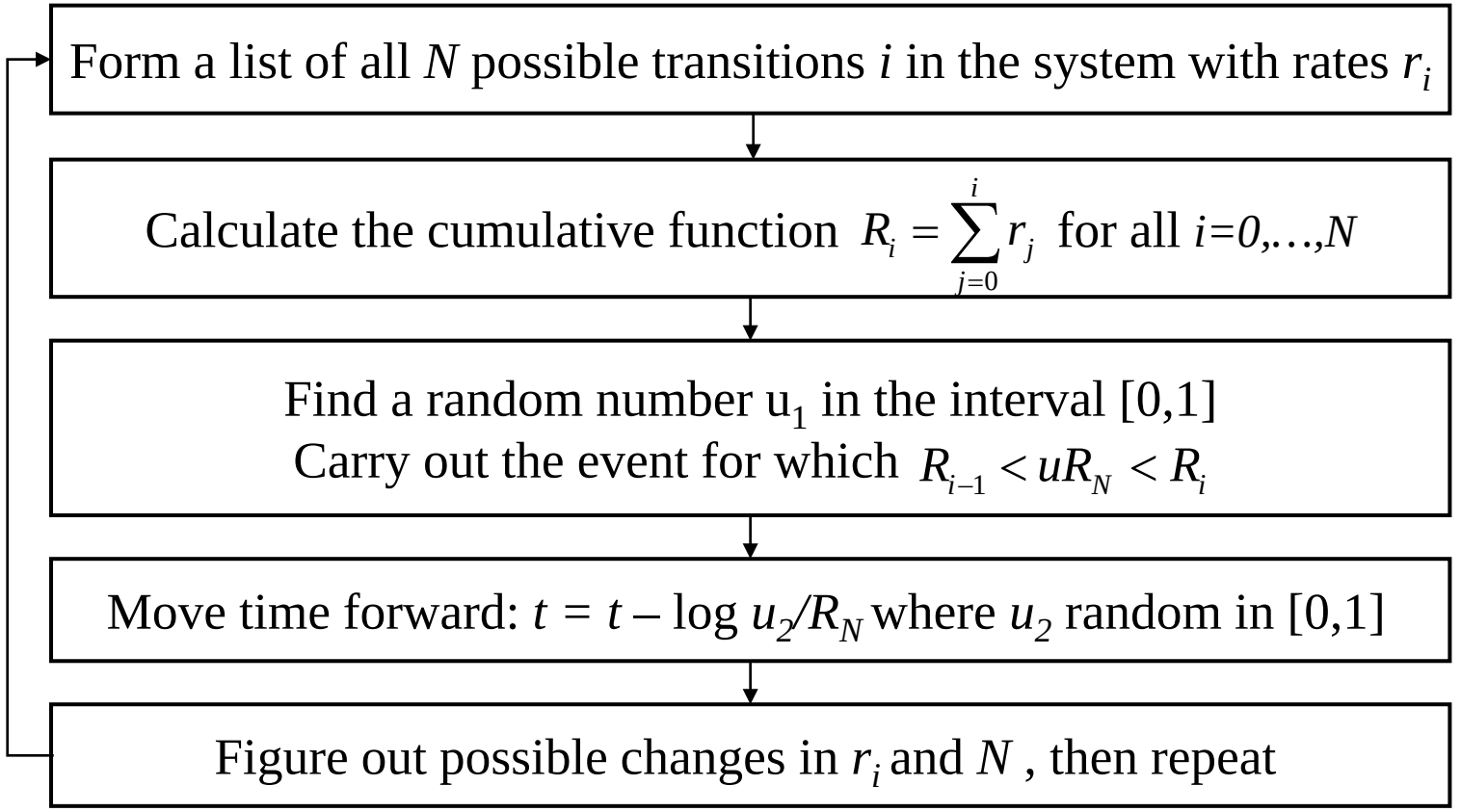
Since the experimental evidence indicates there is a a complex relationship T_{surf} and $c_{D,}$ and MD overestimates fluxes, we took on the following multi-scale approach:

a) To get the long term evolution of D in Be:

use KMC to get <u>equilibrium D profiles in Be</u>

b) Use KMC outcome to get surface D concentration for non-cumulative MD runs, to get more accurate structures and yields

Kinetic Monte Carlo method



Kinetic Monte Carlo method: comments on algorithm

- The KMC algorithm is actually exactly right for so called Poisson processes, i.e. processes occurring independent of each other at constant rates
  - "Stochastic but exact"
- Typical use: atom diffusion: rates are simply atom jumps
  - Ion impact on surface is also a process with a rate!
- But the big issue is how to know the input rates r_i ??
  - The algorithm itself can't do anything to predict them
  - I.e. they have to be known in advance somehow
- From experiments, DFT simulations, …
- Also knowing reactions may be difficult
- Many varieties of KMC exist: object KMC, lattice object KMC, lattice all-atom KMC, …
  - For more info, see wikipedia page on KMC (written by me ☺)

Method

Step 1: OKMC

- In practice, took into use the Open source MMonCa code [1]
- Implemented into this for Be:
  - D implantation
  - Diffusion
  - Cluster formation
  - Trapping / detrapping
- Objects are vacancies V , H/D, carbon C, HV (hydrogen-vacancy complex) and their clusters

[1] I. Martin-Bradado et al. Computer Physics Communications 184 (2013) 2703

OKMC

Parametrization for Be

- Migration and dissociation follow:

$$\nu = \nu_0 \exp(-E^{activation}/k_B T)$$

- Tabulated values for parameters needed for all objects (DFT data):
  - Binding energies for H_nV and H_nC
  - Migration energies
  - E_A = binding E + migration E for dissociation from cluster

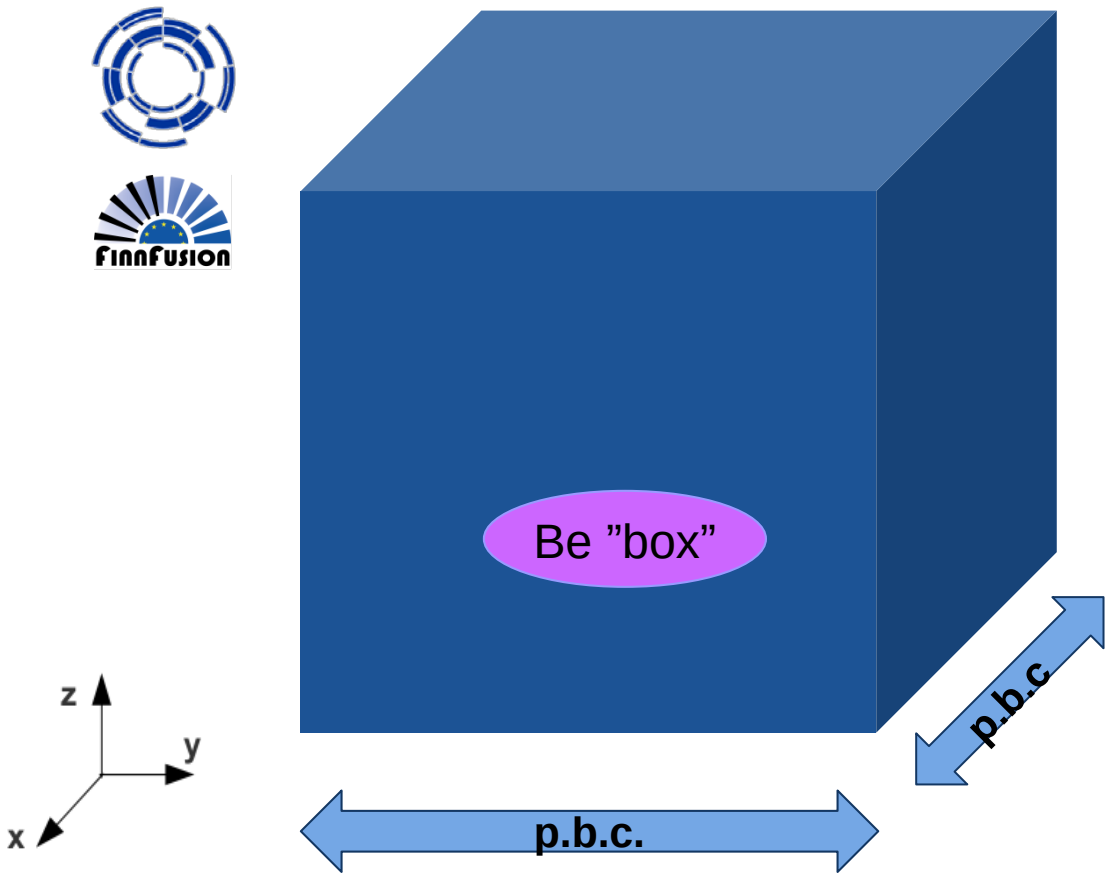
- Parameterization

	$E_{migration}$ (eV)	$E_{formation}$ (eV)
V	0.89 [9]	0.96 [10]
H	0.6 [11]	0.88 [12]
H-V	1 [9]	0.85 [13]
C	0.76 [from NBE]	0.4

[9] Martin-Bragado et al., 2013
[10] S.C. Middleburgh et al., A. Materiala 59 (2011)
[11] M.G. Ganchenkova et al., PRB 75 (2007)
[12] A. Allouche et al., J. Phys. Chem. C 114 (2010)
[13] Calculated within the code
[From NBE]: Elnaz Safi parcas-NEB calculation

OKMC

Setup



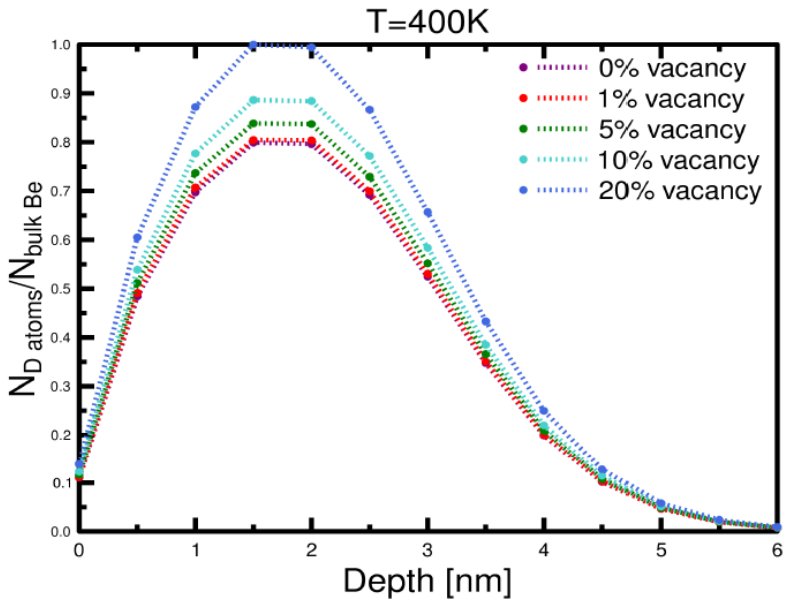
Simulation details:

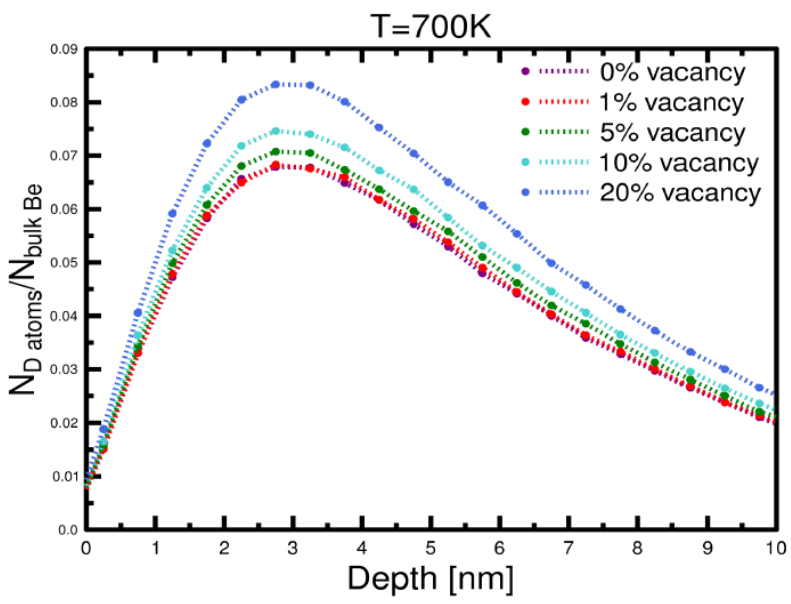
- Box size: 10 * 10 * 100 nm
- Mesh: 0.5 * 0.5 * 0.5 nm
- T = 300, 400, 500, 600, 700 and 800 K
- H Flux ~ 10^{18} $cm^{-2}s^{-1}$
- Impurity concentration = 1% C
- Vacancy concentration (c_V) = 0, 1, 5, 10 and 20%

OKMC

Results

Depth profile of D for different vacancy concentration:



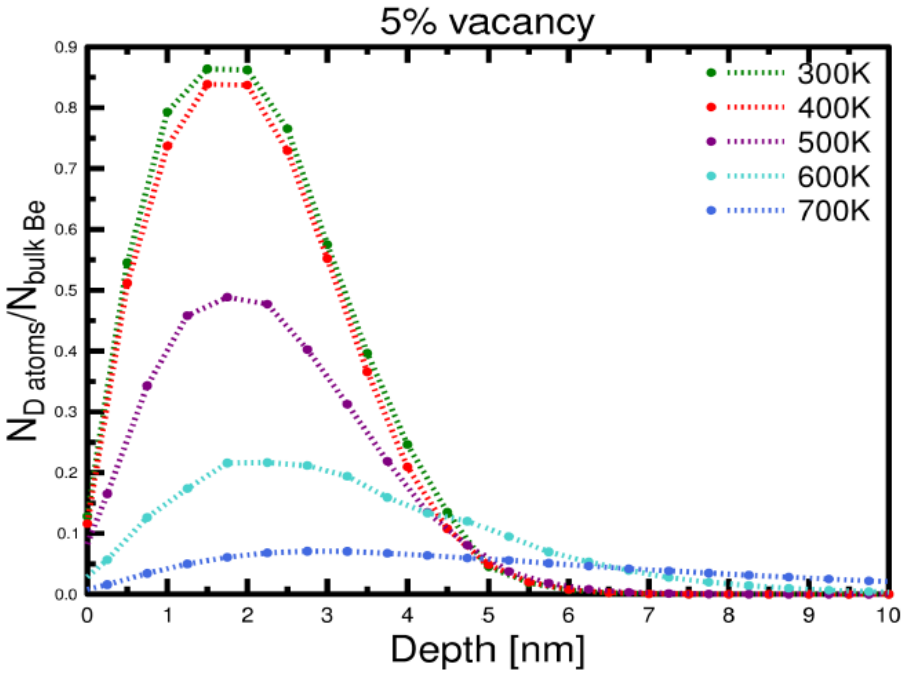


- Almost linear dependence of c_D on c_V
- Profiles varying weakly for c_V ~ 0-10%

OKMC

Results

Depth profile of D for c_V = 5% at different temperatures :



- Final profiles used to set up accurate substrate structure in MD for c_V = 5%
- Also reasonable for co- and re-deposited layers!

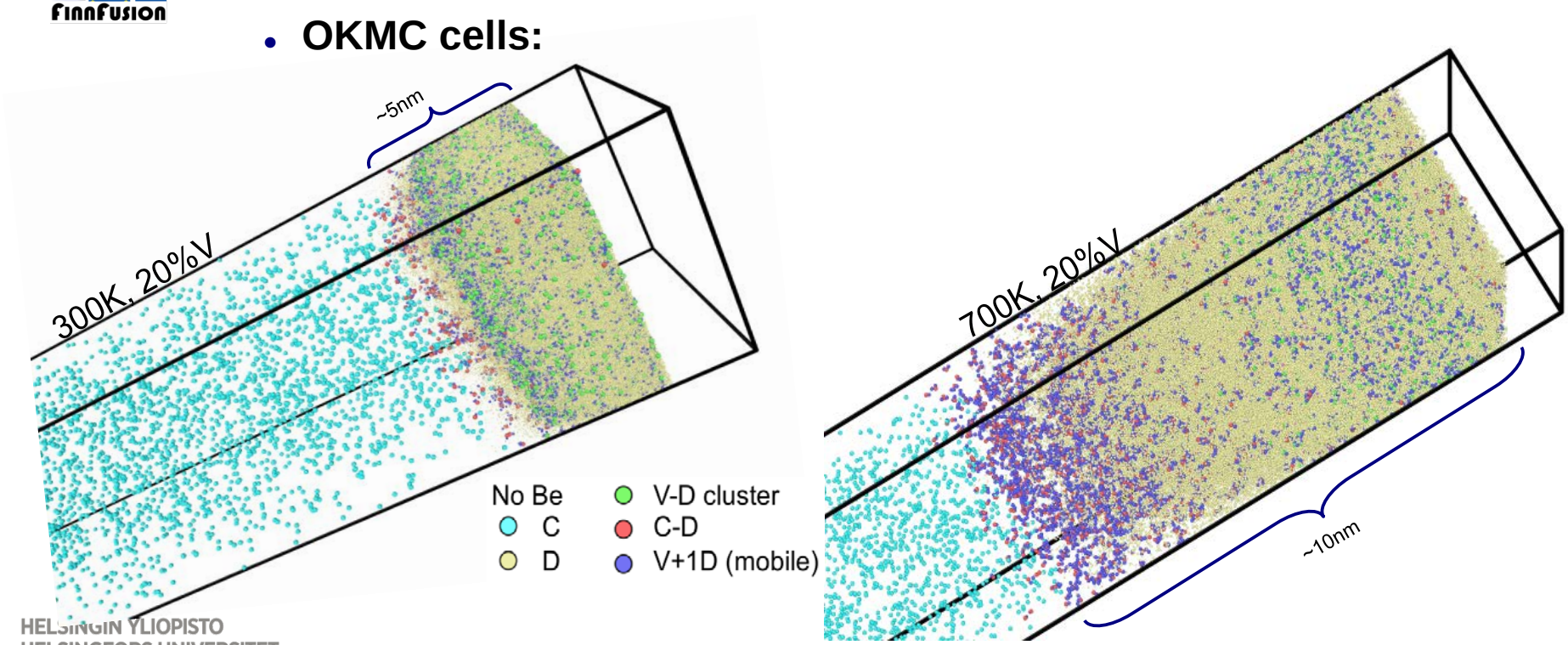
OKMC

Results

- **D trapped per vacancy:**
  - **As in W, more than 1 D per V!**

	300K	400K	500K	600K	700K	800K
1% V	-	5	-	-	4.11	-
5% V	-	5	-	-	4.01	-
10% V	5	4.99	4.99	4.95	3.8	1.32
20% V	5	4.99	4.99	4.95	3.26	1.13

- **OKMC cells:**



Method

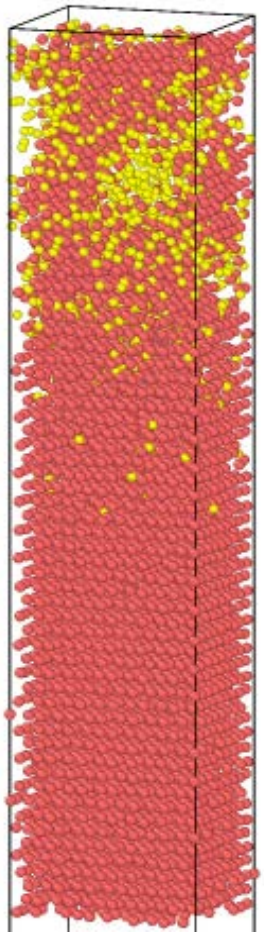
Step 2: MD

Top-to-bottom multi-scaling:

OKMC's output was used to set up accurate substrate structures in MD

MD cell
Be
D

T= 300K



Making the MD structures:

- Instead of a fixed, uniform concentration, use D and V profiles given by OKMC

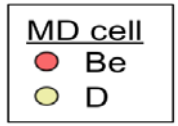
a) Create vacancies

b) Insert D atoms:

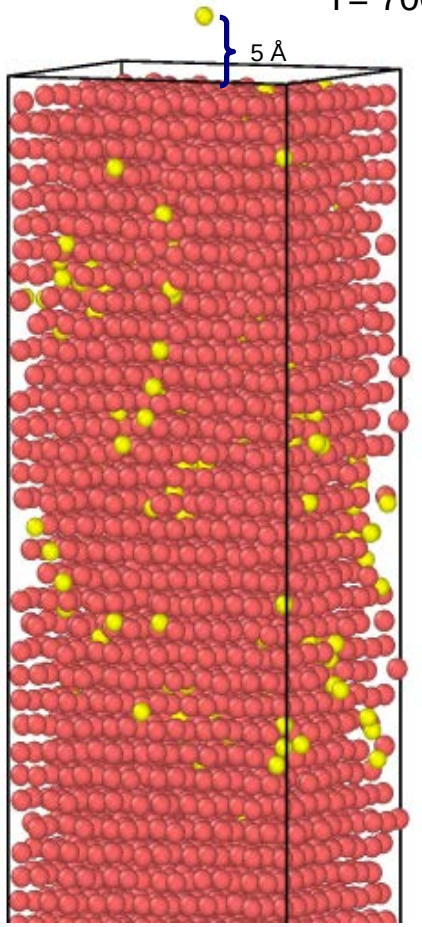
- According to depth profiles
- Accounting for D-per-V results
- Relax the system after each D

MD

Irradiation runs



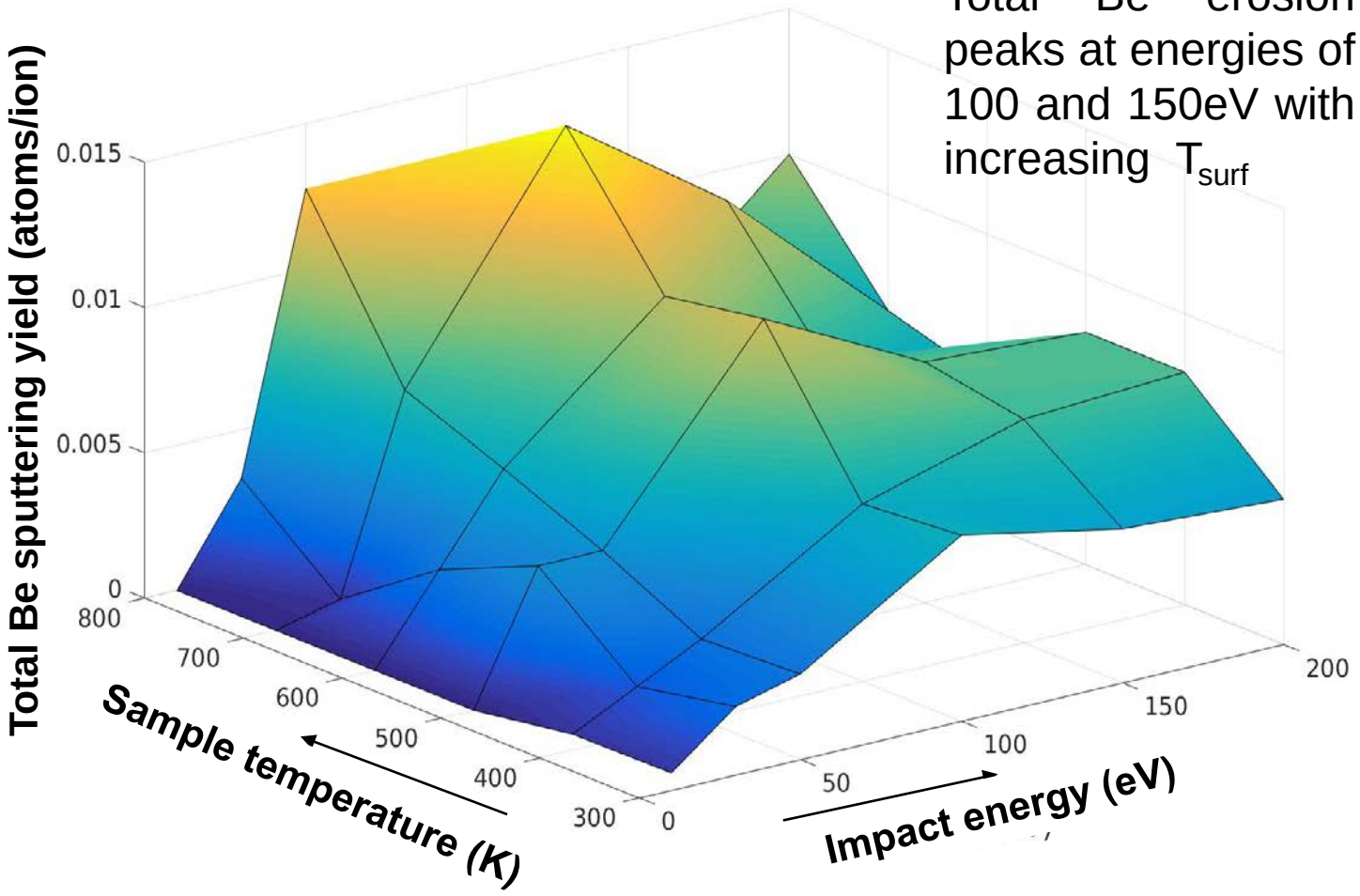
T= 700K



- **D irradiation on Be: non cumulative (static) D impacts**
  - Substrates are ”in equilibrium”
  - Less time consuming: impacts can be run in parallel
  - More controlled conditions: constant c_D/substrate morphology
  - E_i = 10, 30, 50, 100, 150 and 200 eV
  - T = 300, 400, 500, 600, 700 and 800 K
  - Normal impacts to the surface, initiated 5 Å above the surface
  - Cell size: 2 * 2.4 * 12.0 nm
  - Periodic boundary conditions in x, y dimensions

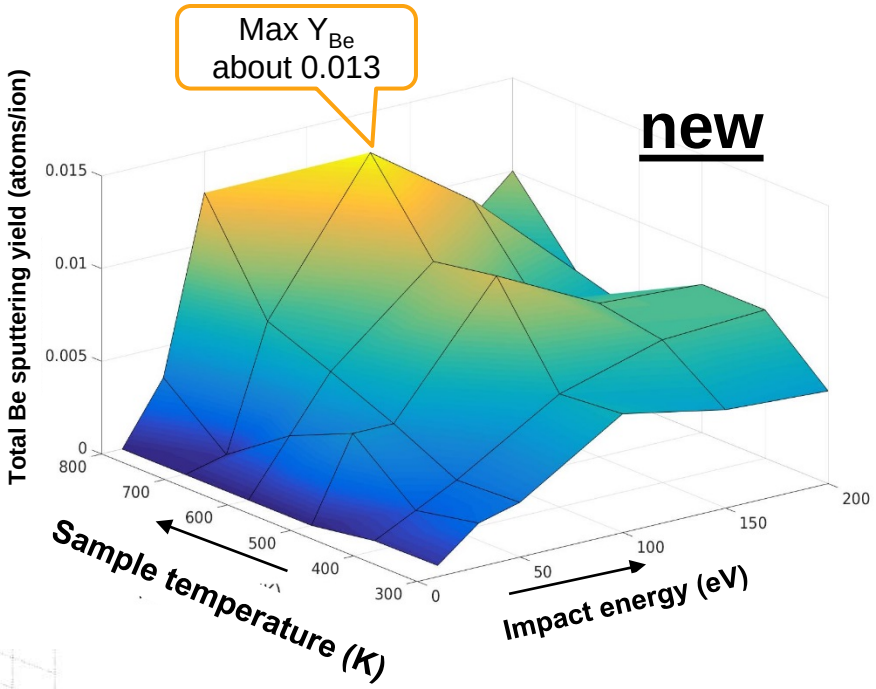
MD fed by KMC:
Results

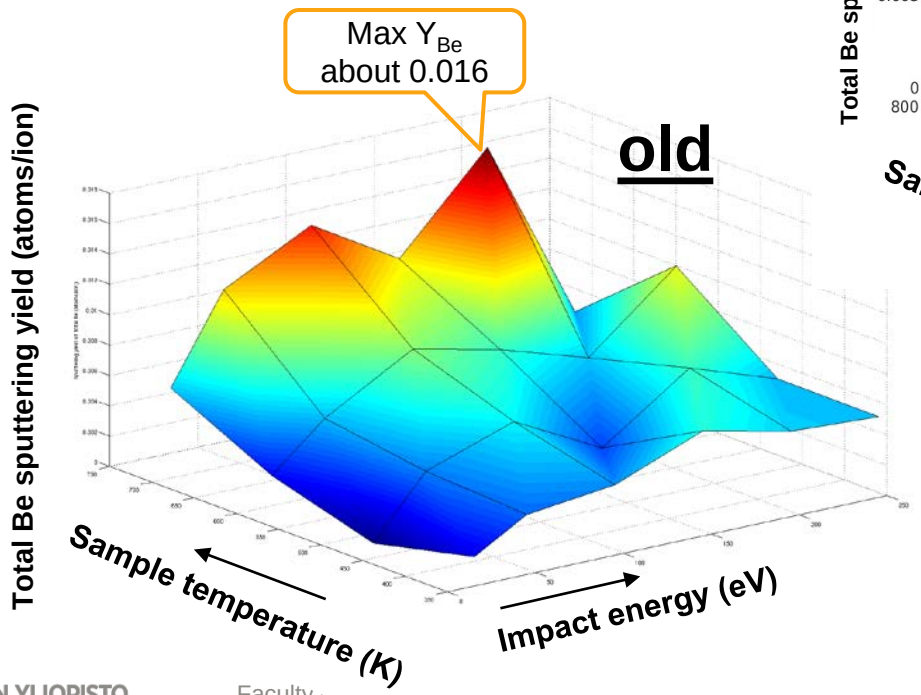
Total Be erosion peaks at energies of 100 and 150eV with increasing T_{surf}



Comparison of old and new results

- Somewhat lower yields with better D surface concentrations
- Maximum at different energy



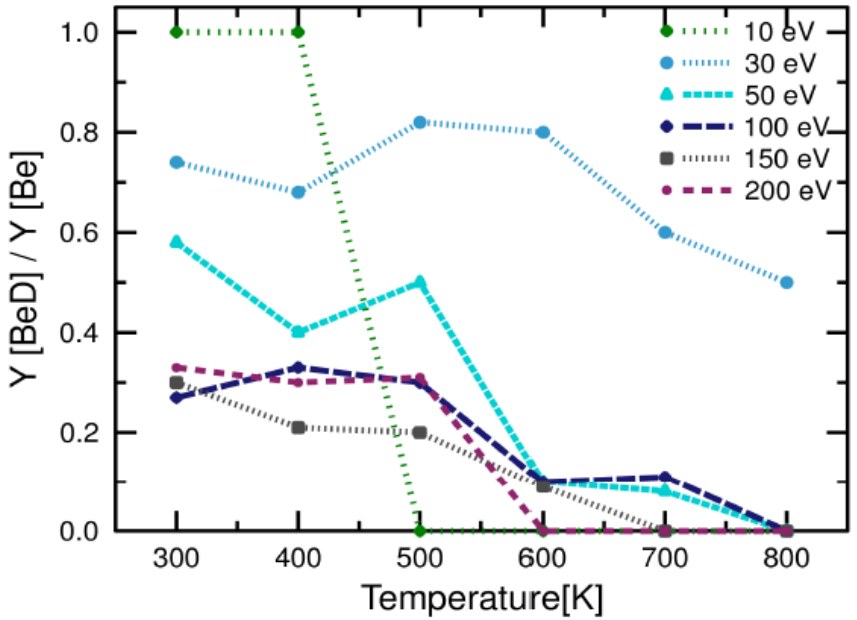


MD fed by KMC:

Results

The fraction of Be atoms that are sputtered as Be molecules:

- In agreement with JET results [2]: the fraction of Be eroded as BeD decays with increasing T_{surf}
- At T_{surf} < 600K and E < 100 eV, the main eroded species is BeD!



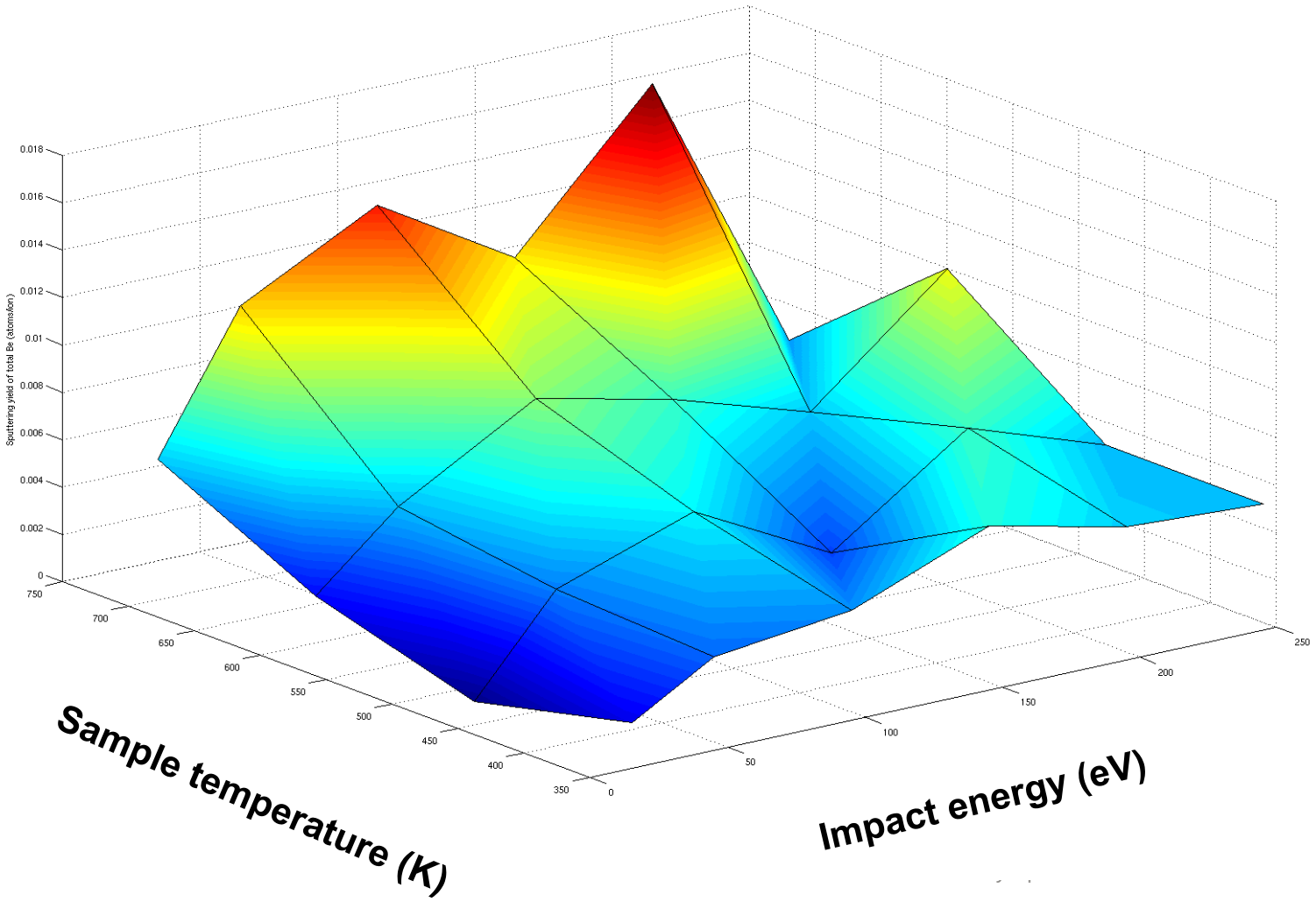
[2] S. Brezinsek et al., NF 54 (2014) 103001

Summary and TODO:

- OKMC code parameterized for Be (first time ever!)
- OKMC results show a linear dependence of c_D on c_V
- At lower T, vacancies are filled with D atoms (up to 5), while at higher T, D atoms detrap from vacancy and occupy an interstitial site.
- MD results are quite sensitive to D content at the surface and T_{surf}
- → Continue the D bombardment on Be cell : at least 3000 impacts
- → Compare data to earlier cumulative T_{surf} scans

Backup slides

D on Be non-cumulative run results: Total Be yield (Energy, Temperature)



D on Be non-cumulative run results: Total Be yield (Energy, Temperature)