EUROfusion

WP PWIE-SP D.D2 T008

Review and Planning Meeting 2022-10-19

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Motivation & Overview

- **Task: (Fast) Erosion modelling considering roughness and morphology for PWI**

  - Which code basis to use?
  - Accelerated modelling using surrogate models : beyond impact angle approximation
  - Gyromotion- and Lattice-structure Effects

I) Code Basis : SRIM vs SDTrimSP

- **SRIM**
  - Based on open-source TRIM-code family (BCA-approximation) and free but is itself **closed-source**
  - Stopping data-base maintained by Ziegler
  - Code is easy to use (GUI, windows), **static targets** only
  - 1-d targets
  - Code results were considered as reliable → SRIM almost de-facto standard: results are used also in this meeting

- **SDTrimSP-family**
  - Based on open-source TRIM-code family (BCA-approximation) and free and **open-source**
  - Developed & maintained mainly by W. Möller, W. Eckstein, A. Mutzke
  - Code is text-file oriented, parallelized (UNIX), static and **dynamic** targets
  - 1-d, 2-d, 3-d target structure

Both are mature, are used almost interchangeable in the fusion community, (see e.g. this meeting) - but our results did not match...

I) Code Basis : SRIM vs SDTrimSP

- **‚Verification‘ challenging**

  - Comparison between SRIM-2013 and SDTrimSP: Differences were obvious – but :
    - Could be due to already known problems (e.g. lack of energy conservation in full cascade mode of SRIM)
    - Difference does not ‚prove‘ that SRIM is wrong: Could be due to either (or both) of
      - Algorithmic differences (e.g. when to subtract energy loss) or
      - Problems in SDTrimSP

  - Many checks were impossible because output of SRIM is incomplete
    - All sub-threshold events are suppressed
    - Collision cascades do not have generation information (ie. assignment is virtually impossible)

      e.g. overflow failures occure silently

⇒ Check for internal (physical) inconsistencies

I) Code Basis : SRIM vs SDTrimSP

- **Simulation results**
  - Good agreement between SRIM and SDTrim depth profiles : **stopping no issue**
  - Discrepancy centered on **replacement** profiles

➡ Design test cases dedicated this aspect :

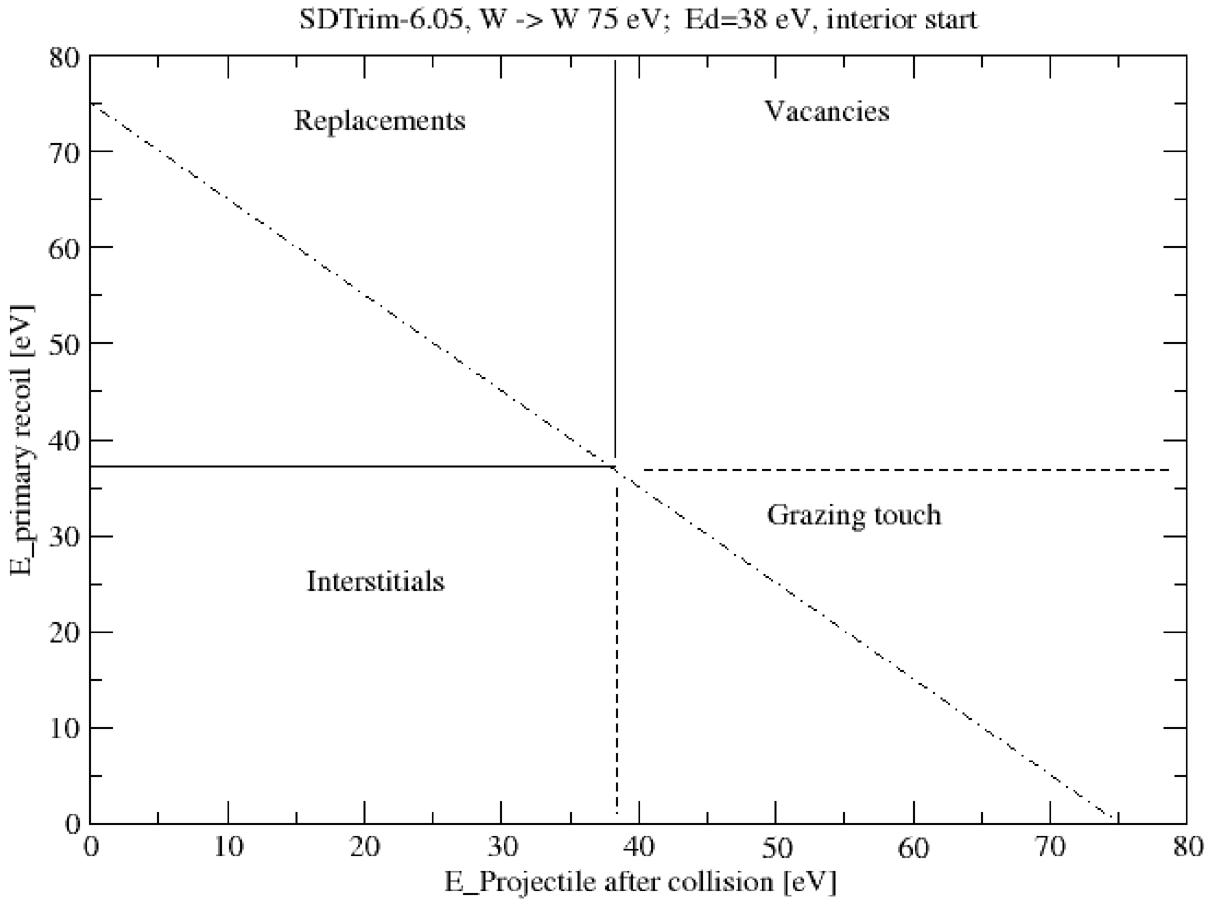
e.g. W → W (homogenious case),

E_0 **= 75** eV initial energy (= 2*38 eV- 1 eV),

E_d **= 38** eV displacement energy,

Angle: 0 degrees

Projectile: interior start

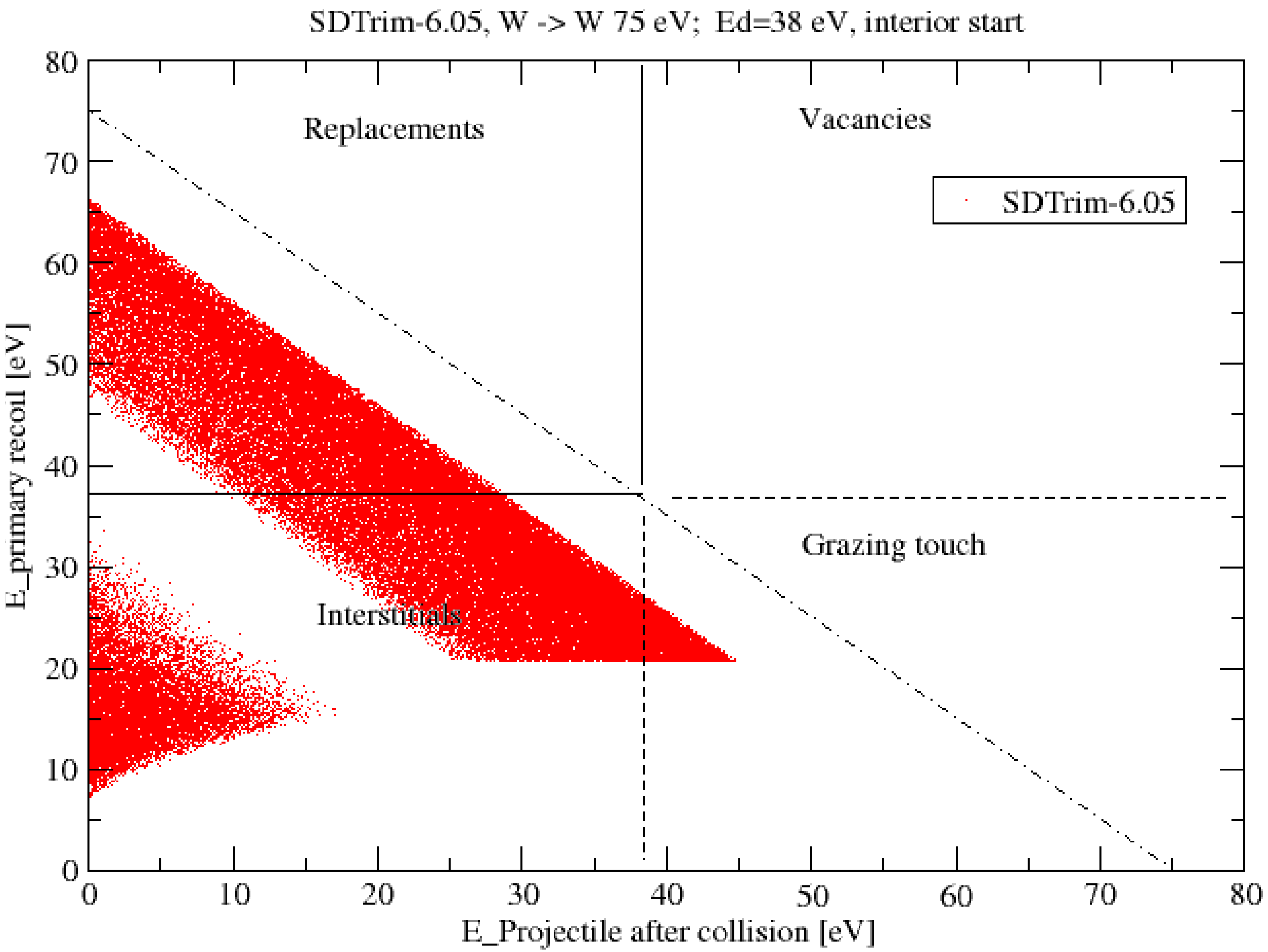


I) Code Basis : SRIM vs SDTrimSP

- **Simulation results: SDTRIM**

Some notworthy features:

- Minimum energy transfer
- Gap in energy density
- Bulk binding energy

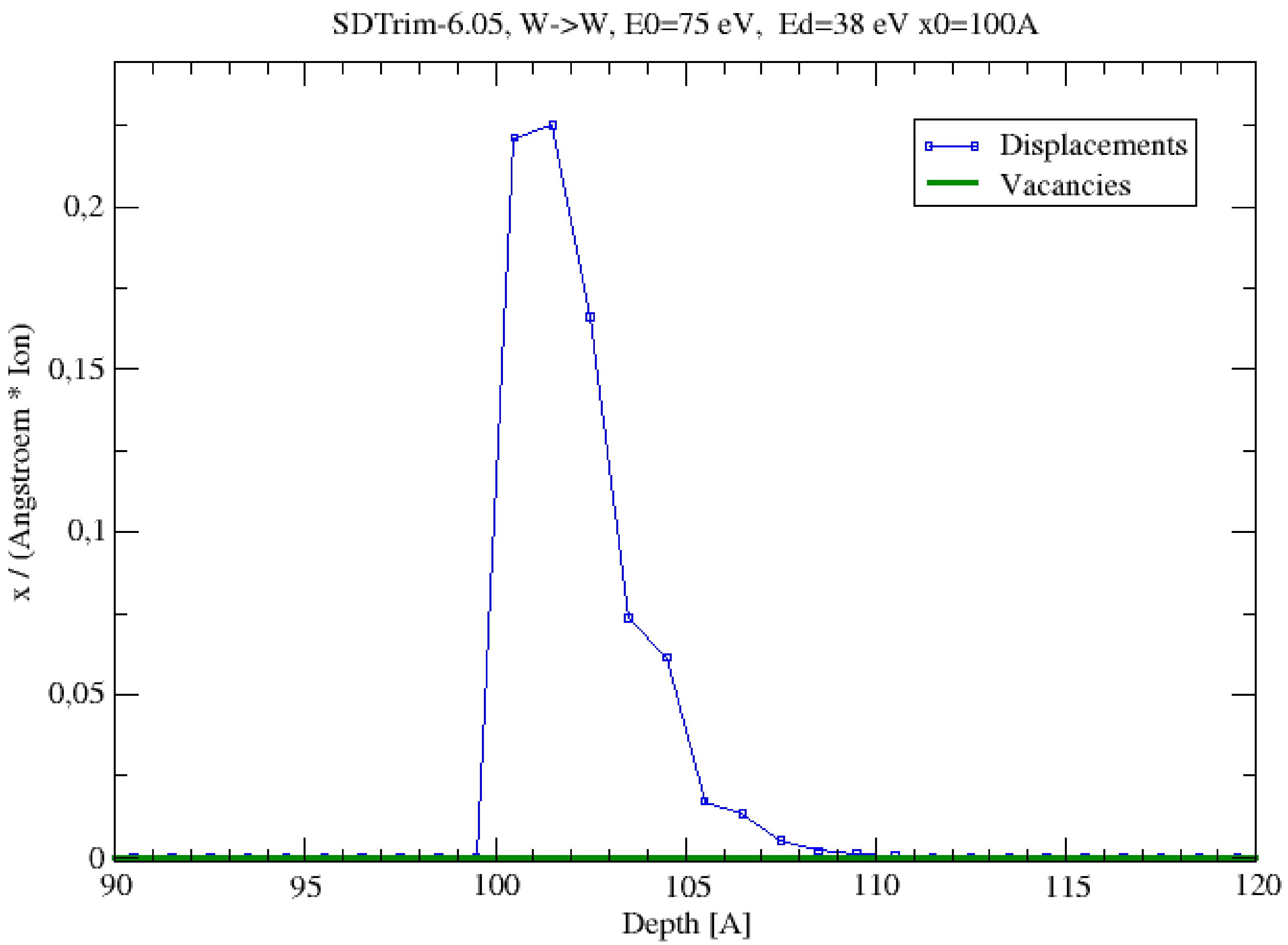


I) Code Basis : SRIM vs SDTrimSP

- **Simulation results: SDTRIM**

Some notworthy features:

- No vacancies (as expected)
- All *displacement* events are **replacement** events
- Only interstitials are present



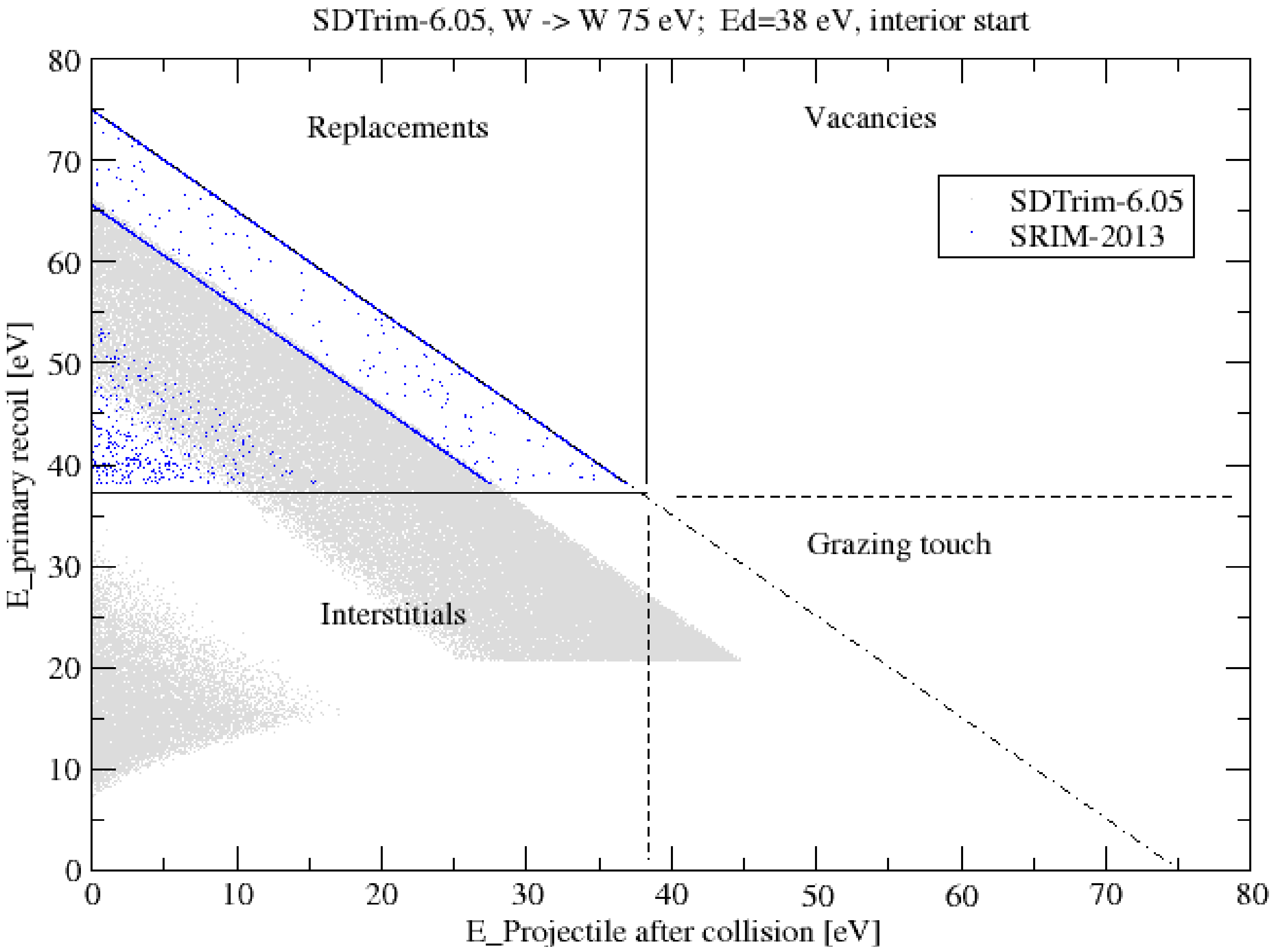
I) Code Basis : SRIM vs SDTrimSP

- **Simulation results: SRIM**

Some notworthy features:

- Discrete structures
- Incomplete output
- Bulk binding energy ?

→ General agreement
- appears reasonable.



I) Code Basis : SRIM vs SDTrimSP

- **Simulation results: SRIM**

Some notworthy features:

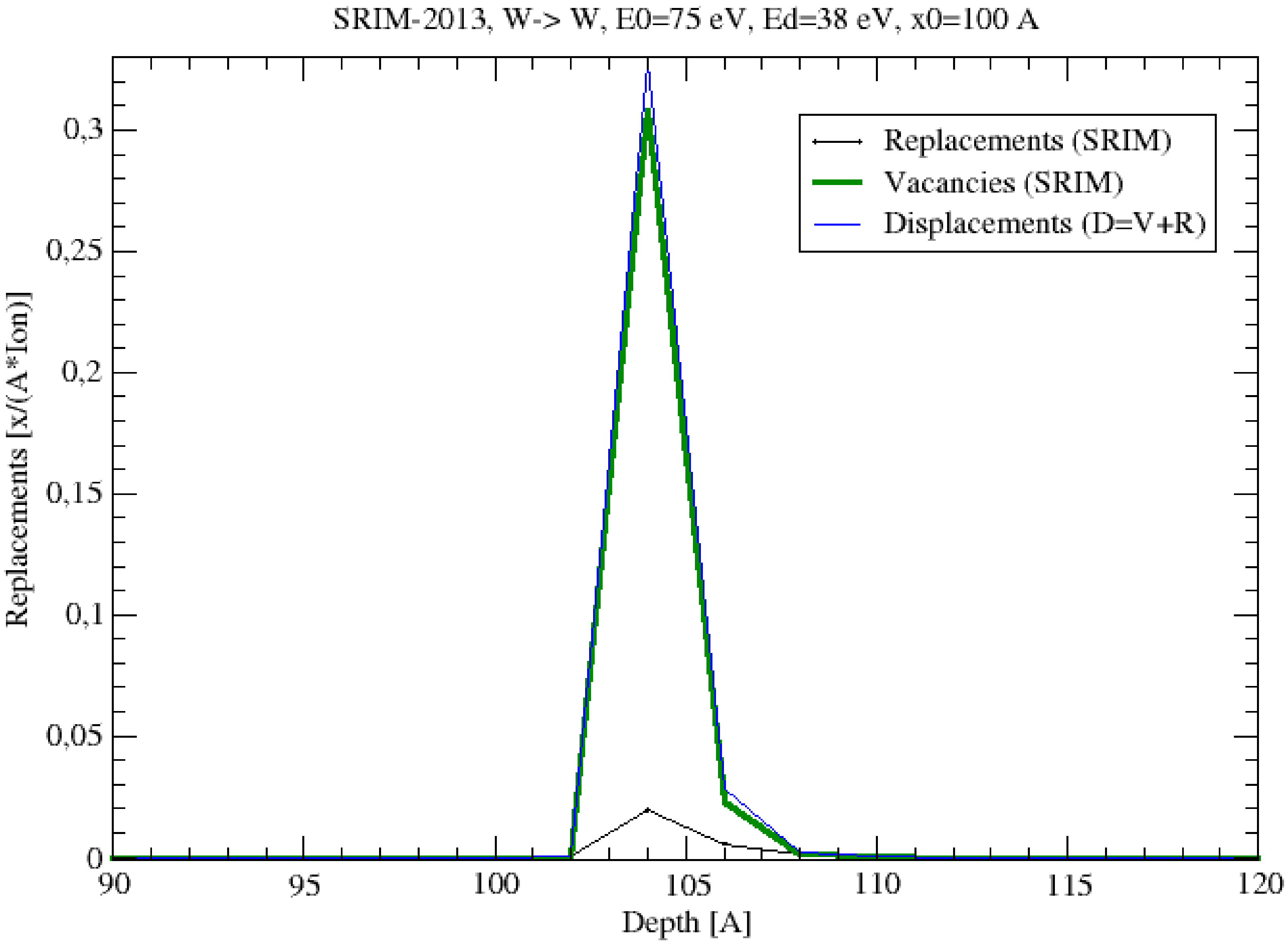
- Phase space yields:

  no vacancies are present

- Output:

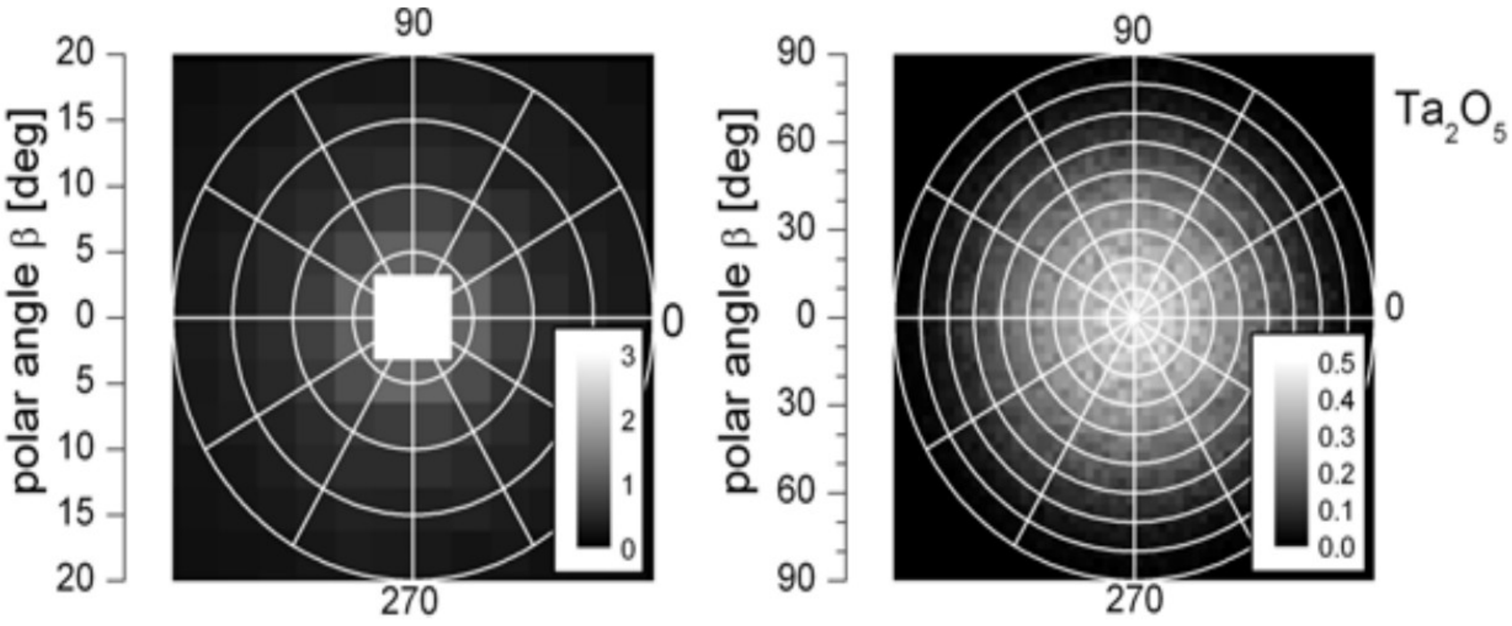
  Dominantly vacancies

➡ SRIM-code information on *Replacements* and *Vacancies* and thus *displacements (sum)* is **wrong!**

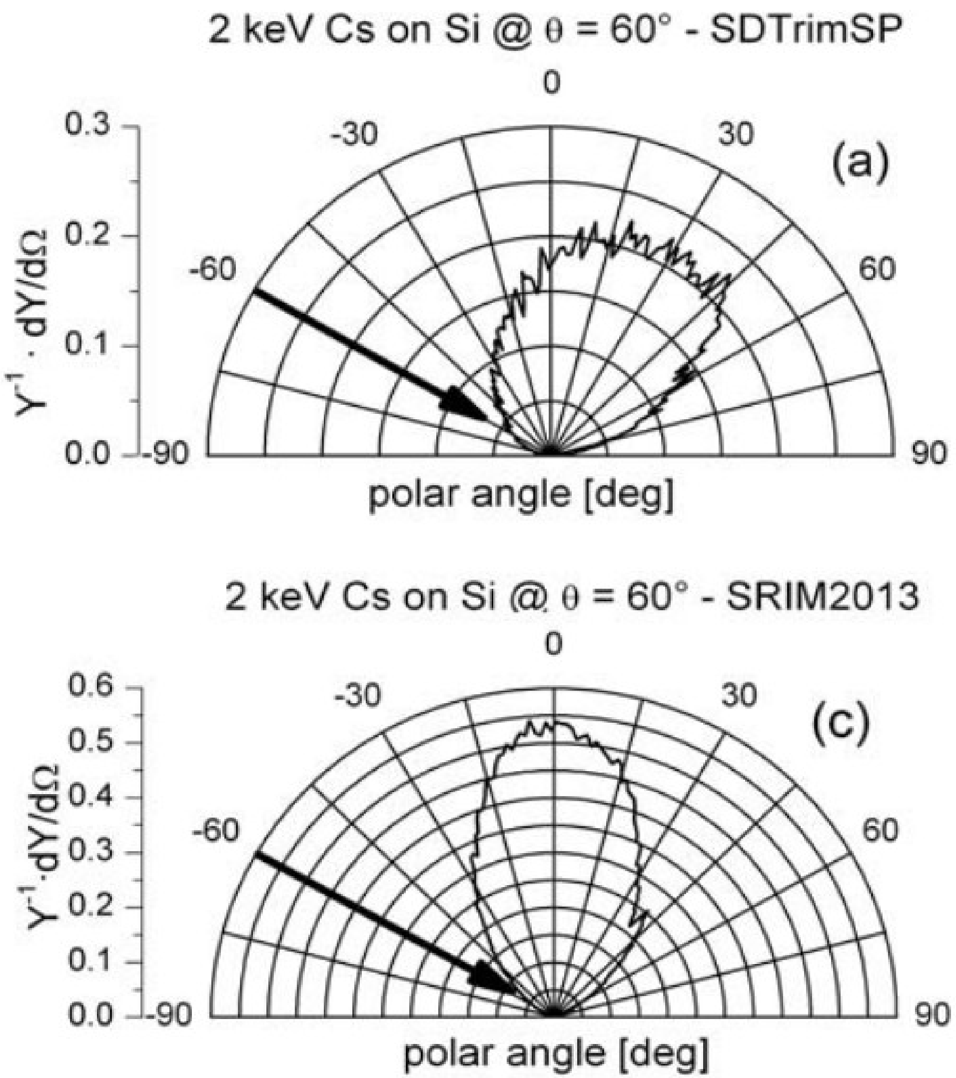


I) Code Basis : SRIM vs SDTrimSP

- **SRIM**
  - Hofsäss et al Appl. Surf Sci 310 (2014),
  - p. 134-141 : Angular sputter distributions are wrong
  - Perpendicular emission for some ion-target comb. (Z<14)



1 keV Ar



I) Code Basis : SRIM vs SDTrimSP

- **Summary :**

- Stopping (range) calculations do agree in the considered cases

- Some algorithmic differences between SDTrim and SRIM (when/how is energy loss accounted for)

- Output of SRIM-2013 with respect to damage is **broken** and **unreliable** and **should not be used**

- All present investigations yield **systematic overestimation** of amounts of **vacancies by SRIM-2008 and SRIM-2013** (c.f. Agarwal, Lin, Li, Stoller, Zinkle, NIMB 503 (2021) p. 11-29 → use full-calculation and hand-edit output)

- Reason for provable wrong sputtering results unknown

- Contacted James Ziegler on that issue but communication stalled (Corona?)

- No internal problems with SDTrim 6.05+ have been found: consistent results, now also GUI available: see P. Szabo et al, NIMB 522, p. 47-53 (2022)

Overview

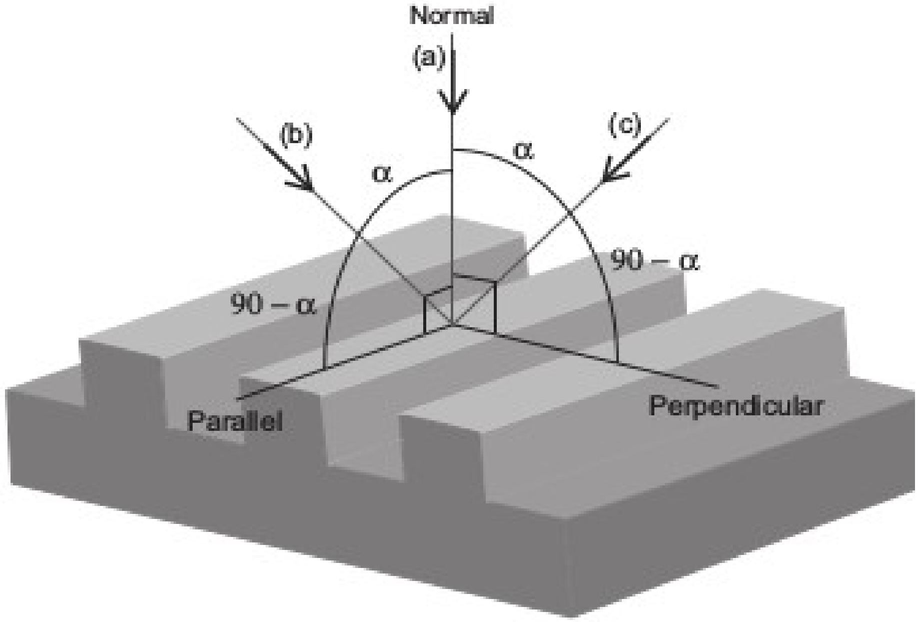
- **Task: Erosion modelling considering roughness and morphology for PWI**

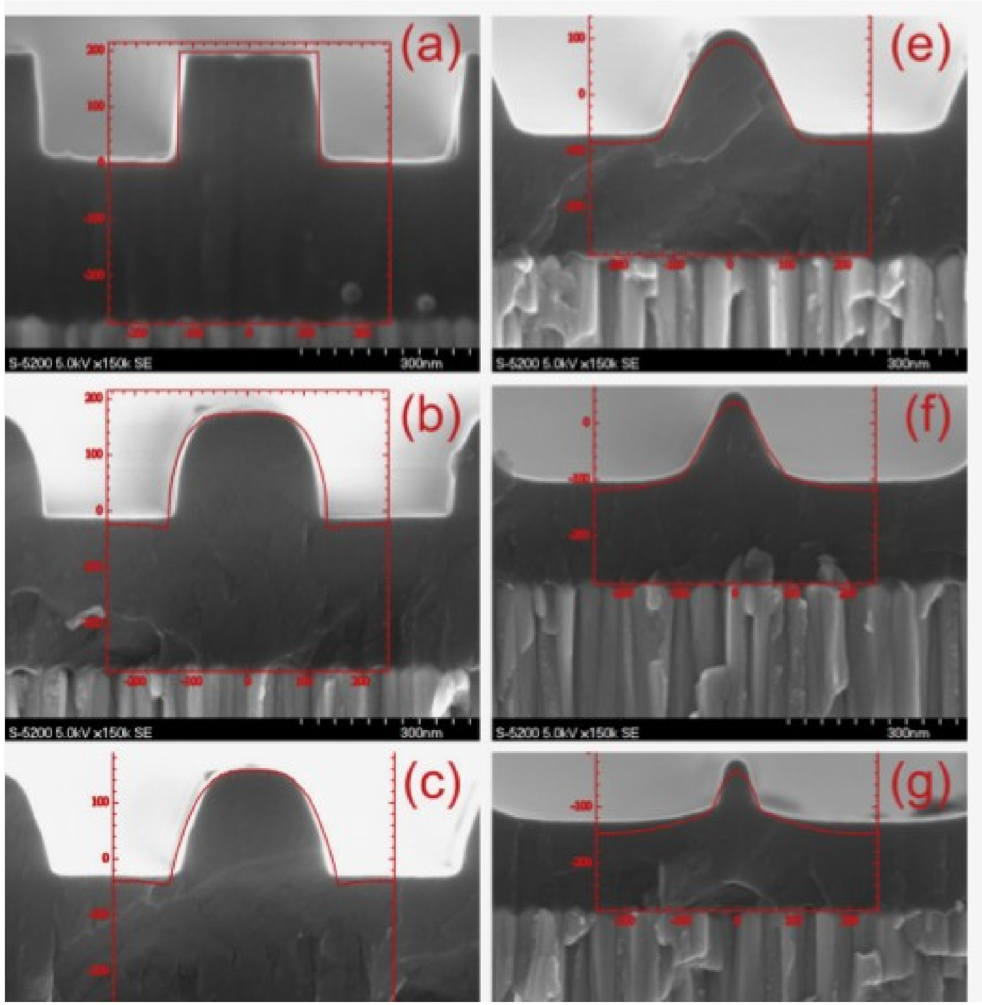
  - Which code basis to use?
  - **Accelerated modelling using surrogate models : beyond impact angle approximation**
  - Gyromotion- and Lattice-structure Effects

II) Accelerated Modelling with Surrogates

- **Dynamic Modelling with SDTrimSP-2D and SDTrim-3D**
- Self-consistent dynamic surface evolution under sputtering processes
  - in 2D and 3D

1) Codes are validated against experimental results (predictive simulations!)

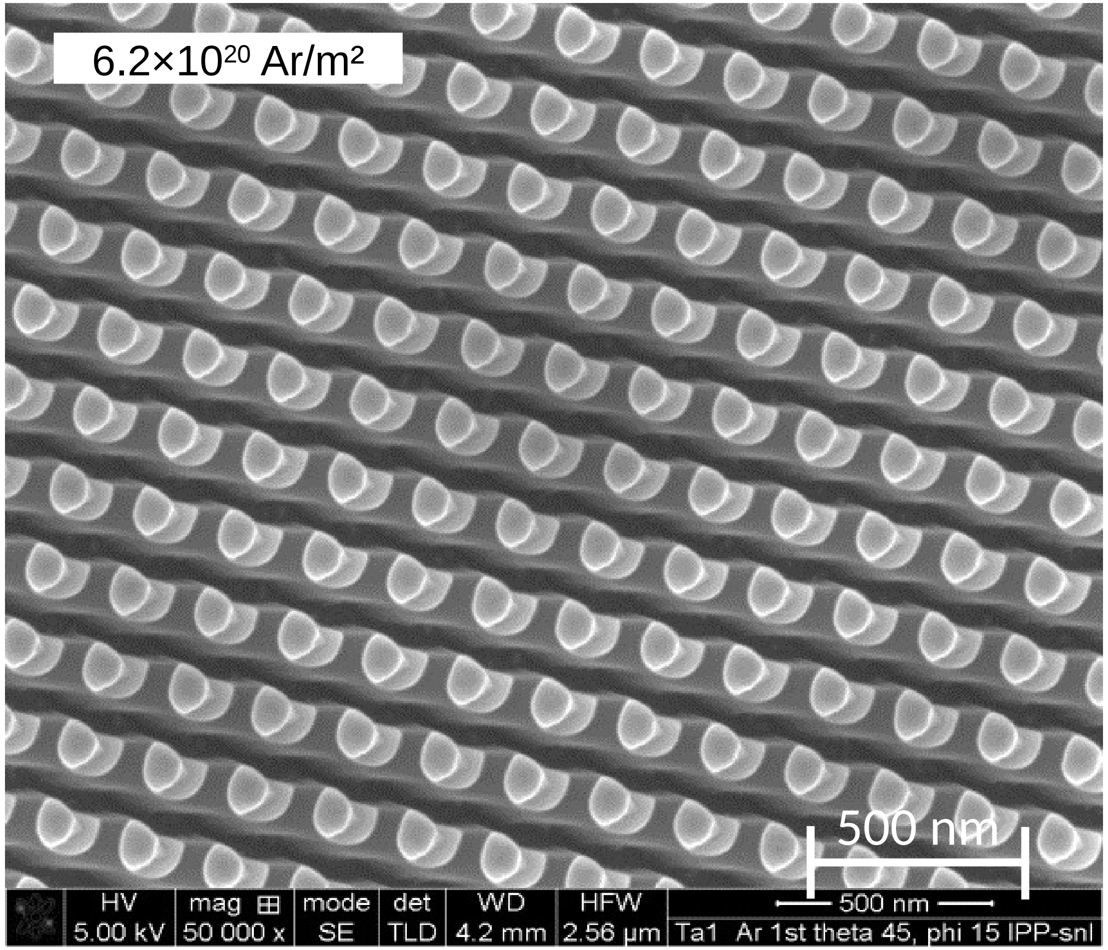


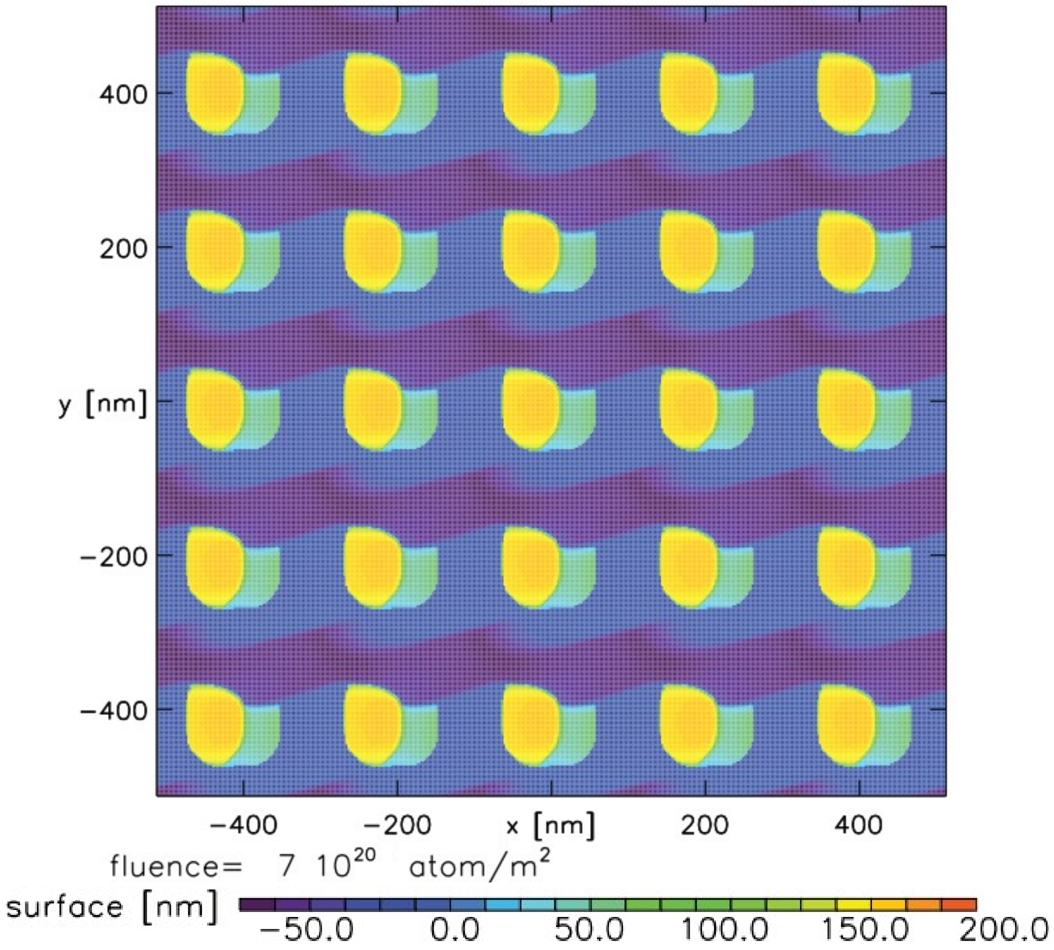


I. Bizyukov, A. Mutzke, R. Schneider, J. Davis. Evolution of the 2D surface structure of a silicon pitch grating under argon ion bombardment: Experiment and modeling. NIM-B, 268 (2010)

Ta – 45° incidence, 15° rotation

SDTrimSP-3D Ta columns eroded by 5 keV Ar under 45° incidence, 15° rotation





II) Accelerated Modelling with Surrogates

Dynamic Modelling with SDTrimSP-2D and SDTrim-3D

Self-consistent dynamic surface evolution under sputtering processes in 2D and 3D
Codes are validated against experimental results (predictive simulations!)
Physics complete (within known limits) → computation of reference solutions
Task solved…. Drawback: long simulation times (N^3-scaling)

Sputtering of rough surfaces: acceleration using surrogate models

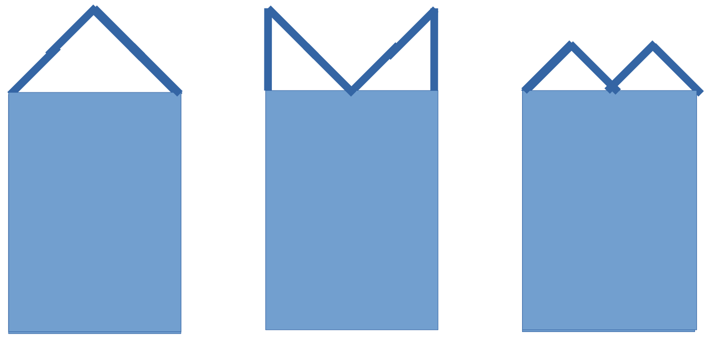
- Well known key parameter: angle of ion incidence **α** [Sigmund, Phys Rev. 184, p. 383 (1969)]
- Many modelling approaches over several decades:
  - Self-similar surfaces: fractal-TRIM (D. Ruzic, NIMB 47, p. 118 (1990))
  - AFM or profilometer-data based angle-distributions, e.g.
    - ’The influence of surface roughness on the angular dependence of the sputter yield’, NIMB 145, p. 320 (1998)
    - ‘Sputtering of rough surfaces: a 3D simulation study’, Physica Scripta T170:014056 (2017)
    - C. Cupak et al, Applied Surf. Sci 570(2021) p. 151204 (this Monday)

- General observation: **reduced** effective erosion, **smoothed** response to incidence angle variations

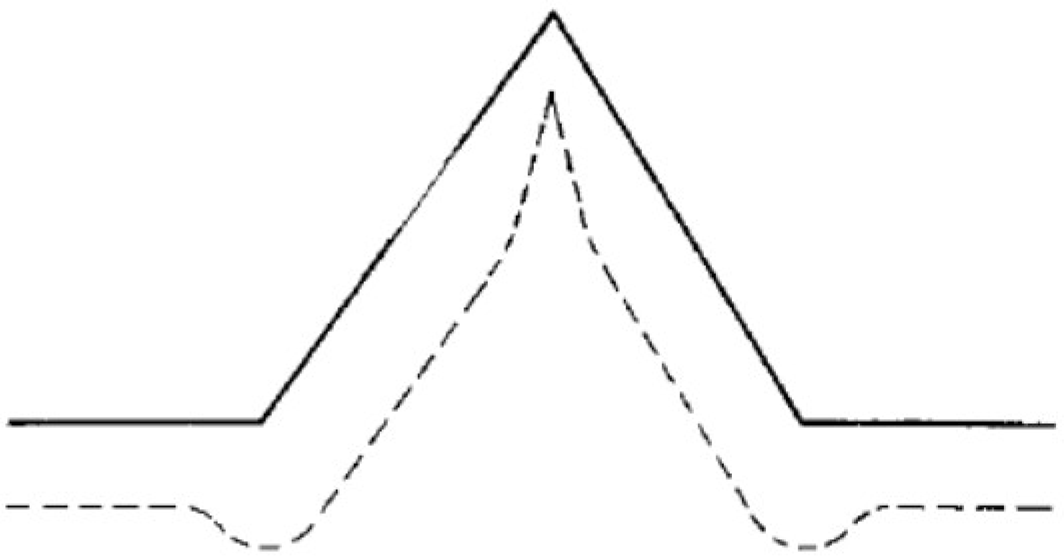
II) Accelerated Modelling with Surrogates

Limitations of impact angle distribution Y(α) as defining parameter

- Incomplete information,
  - e.g. three pillars with **same** impact angle distribution: which one sputters fastest? Need p(**ω**) and p(**ω**,**ω**')



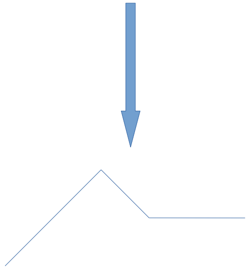
- Theory and Simulation suggest Y(**α**, **α**') instead, i.e.



local surface ***curvature*** affects sputter yield: crucial for dynamics

- P. Sigmund, 'A mechanism of surface micro-roughening by ion-bombardment, J. Mat. Sci. 8, p. 1545 (**1973**)
- M. Wagner et al, 'Simulation of the evolution of rough surfaces by sputtering' , Rad. Effects and Defects in Solids 177, p. 1019 (2022)

II) Accelerated Modelling: beyond impact angle models



SDTrimSP-surrogate (2D) (by R. Preuss):

- Fast ML-based predictor for large-fluence induced morphology changes:
    - initial phase (slow):
        - large-scale cluster-based computation of database (i.e. $Y(\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3)$ instead of $Y(\boldsymbol{\alpha})$)
        - Data from SDTrimSP-Simulations (2D)

    - application (fast)
        - Dynamical iterative predictor for morphology evolution (matrix-vector multiplication)

    - Validation of ML model against 2D-SDTrimSP (and assessment of limitations)

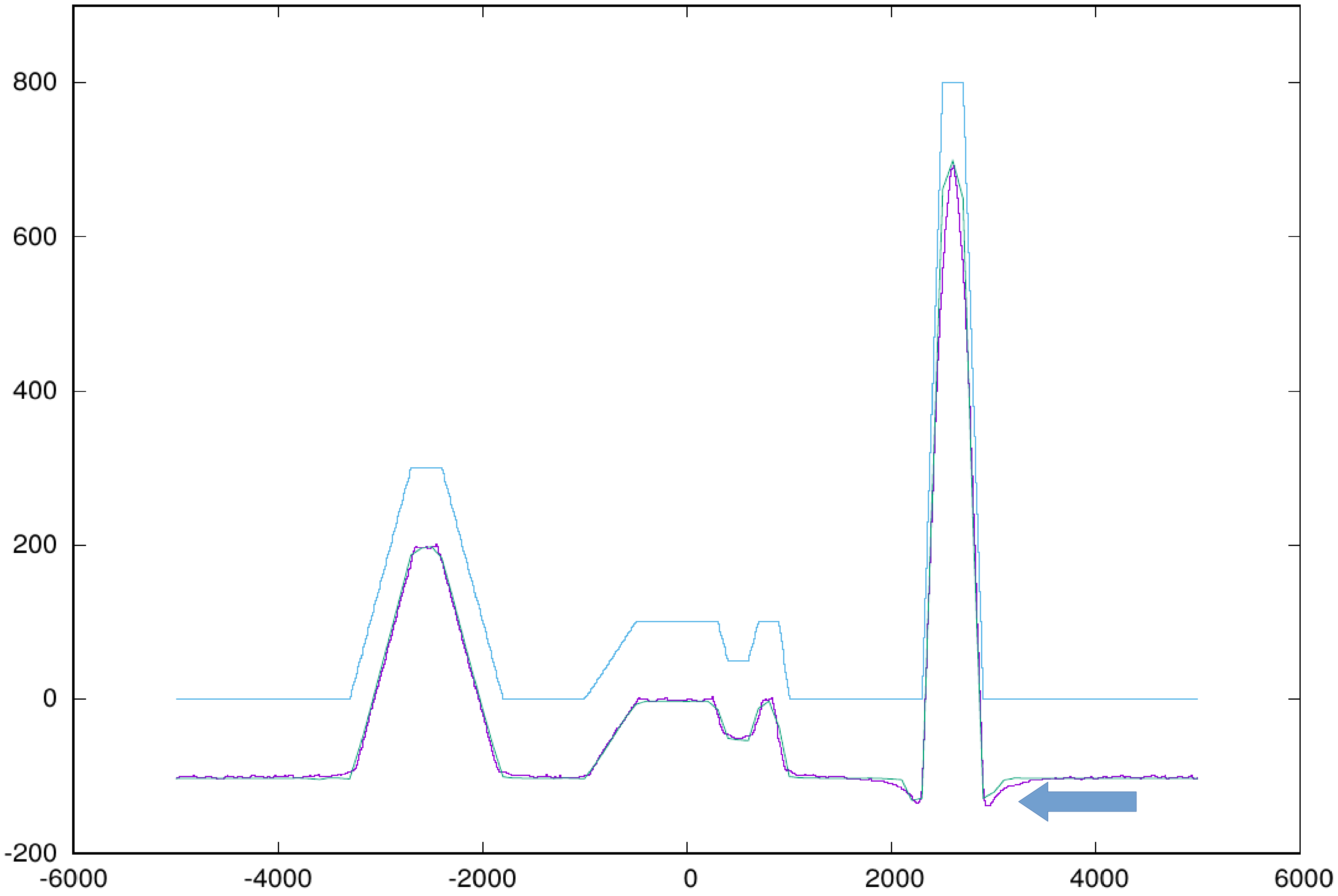
II) Accelerated Modelling: beyond impact angle models

SDTrimSP-surrogate :

5 keV Ar → Cu

Results

- **non-linear effects are retained**
- **acceleration by a factor ~300 (non-optimized)**
- **deviation for α>80 degrees**



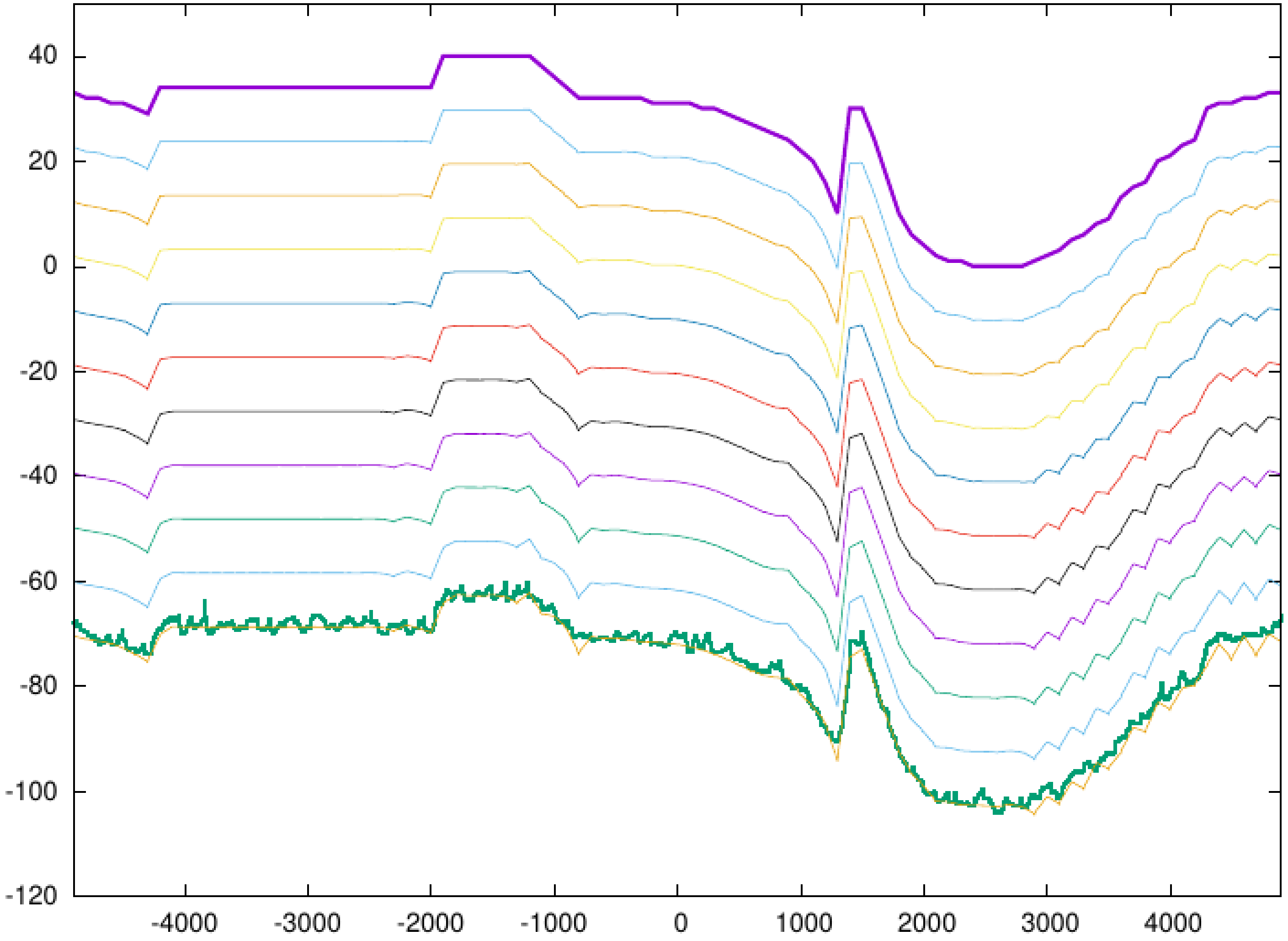
II) Accelerated Modelling: beyond impact angle models

SDTrimSP-surrogate :

Results

- **non-linear effects are retained**
- **acceleration by a factor ~300 (non-optimized)**
- **deviation for α>80 degrees**
- **quantitative agreement with SDTrimSP-2D simulations**

To Do: non-perpendicular impact



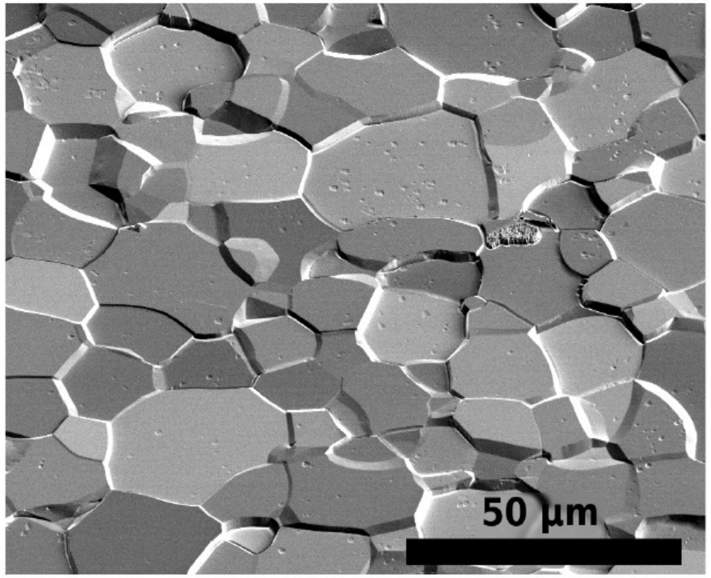
Overview

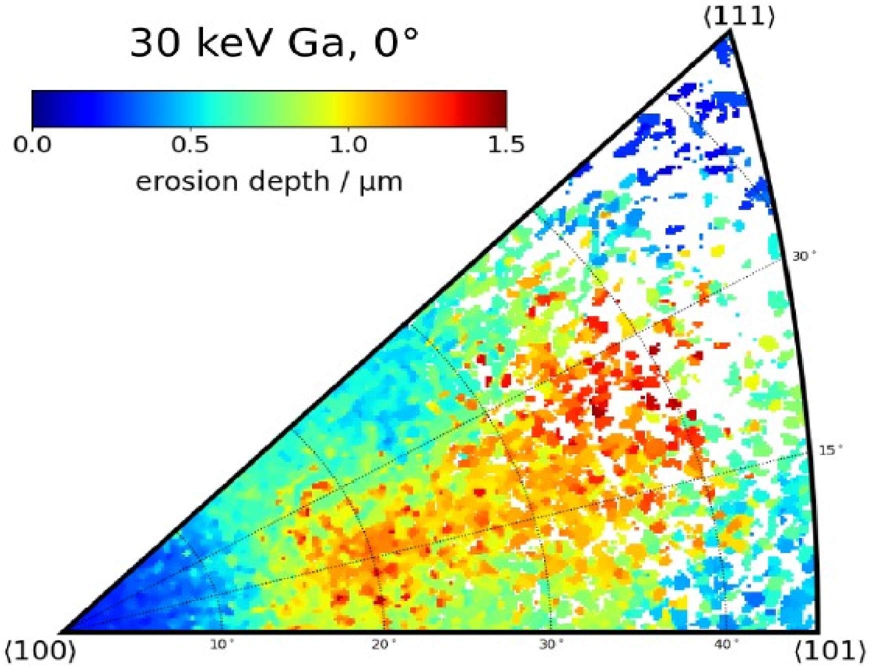
- **Task: Erosion modelling considering roughness and morphology for PWI**

  - Which code basis to use?
  - Accelerated modelling using surrogate models : beyond impact angle approximation
  - **Gyromotion- and Lattice-structure Effects**

Lattice-Structure Effects

- **Sputtering depends on the local atomistic structure**



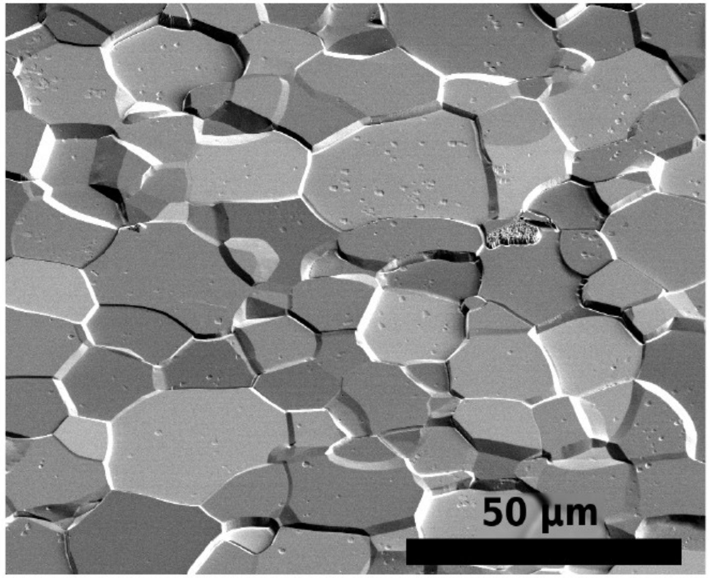


images from PhD thesis Karsten Schlüter (2021)

- Available simulation tools are limited : MD, MARLOWE, ...
- Idea: Enhance SDTrimSP with lattice-capabilities

Lattice-Structure Effects

- **Sputtering depends on the local atomistic structure**



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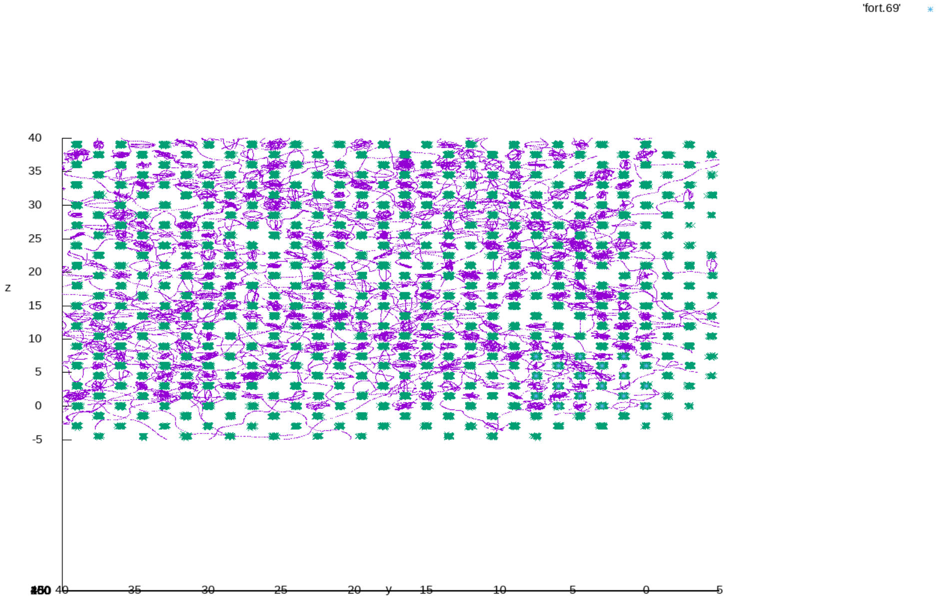
Be on W, 200 eV, channeling



- Available simulation tools are limited : MD, MARLOWE,

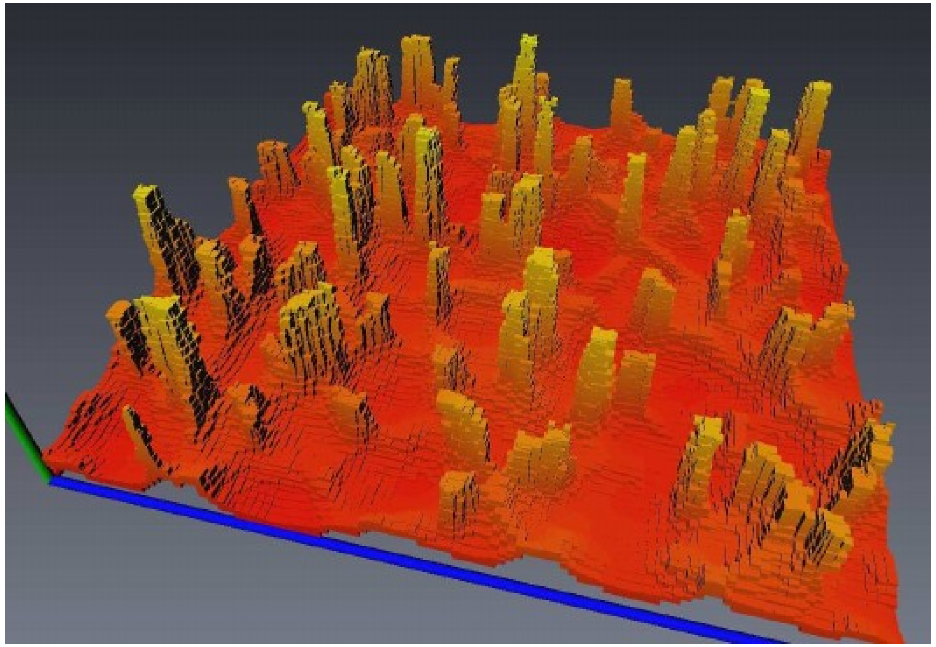
- Idea: Enhance SDTrimSP with lattice-capabilities - Realization: Code presently in final testing stage

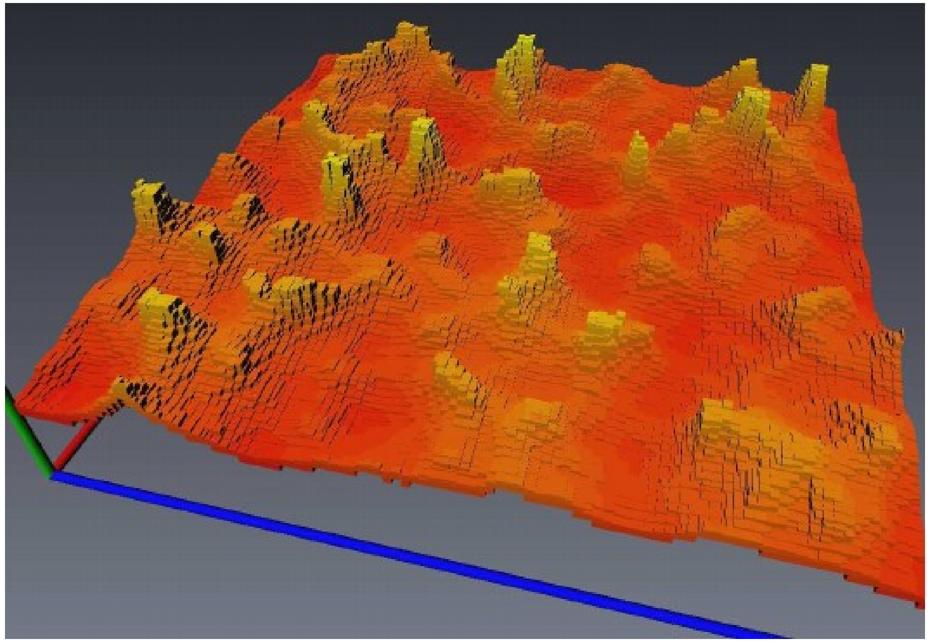
Gyromotion

- **SDTrim-Gyro**
- Influence of magnetic/electric fields on sputtering (re-ionization, gyro-orbits)

B= 0 T   B = 1.1 T

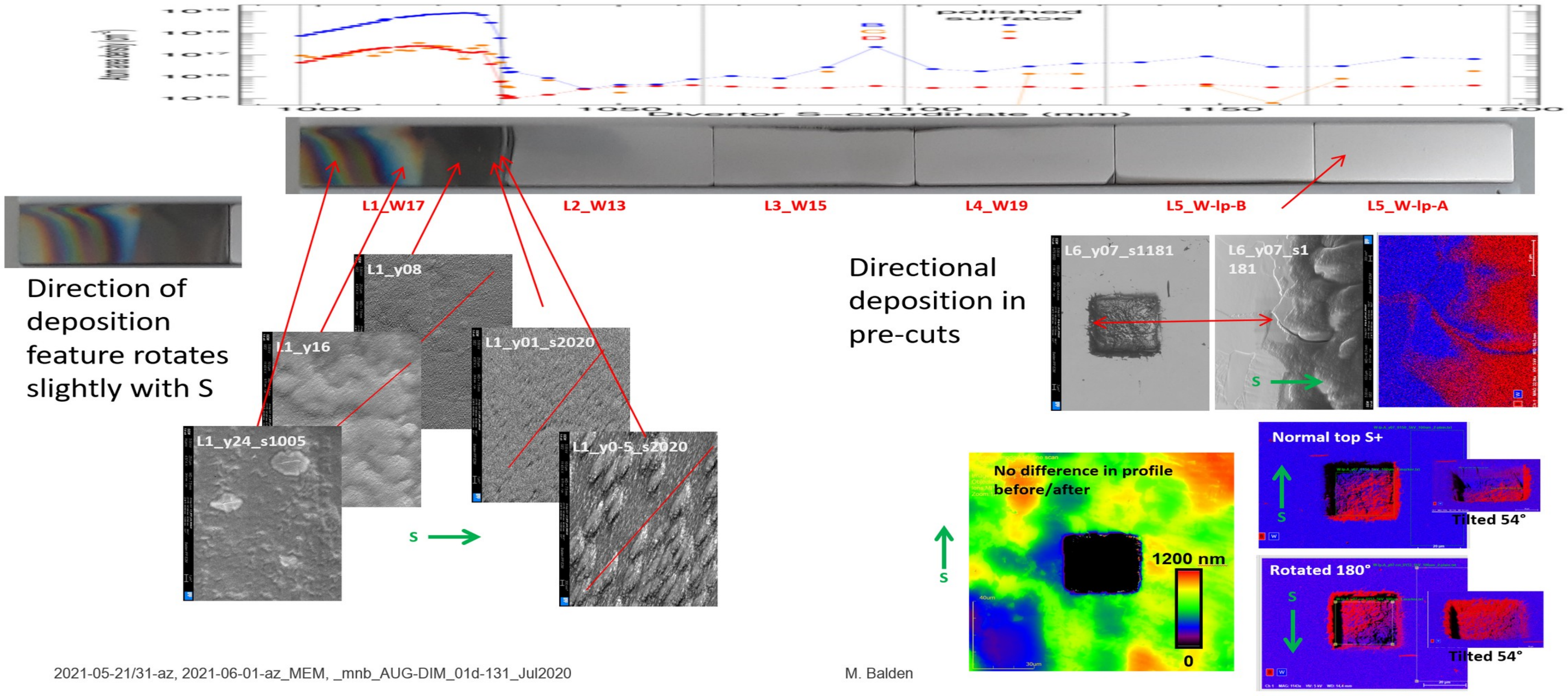
200 eV D on W/Fe sample (**α**=0 deg)





Gyromotion

- **SDTrim-Gyro**
- Exposure of dedicated laser-structured sample (Rodrigo, Balden) : too rough
- *Piggyback* experiment at end of AUG-operation (M. Balden, K. Krieger et al):
- Polished parts appear suited for evaluation
- Evaluation pending...



Summary

- **Task: Erosion modelling considering roughness and morphology for PWI**

  - Which code basis to use? → SDTrimSP

  - Accelerated modelling using surrogate models : beyond impact angle approximation : Y(**α**,**α**')

  - Gyromotion- and Lattice-structure effects

- Thank you very much – Questions?

I) Code Basis : SRIM vs SDTrimSP

Simulation results: SDTRIM

Some notworthy features:

- Minimum energy transfer
- Gap in energy density
- Bulk binding energy