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TSVV7
Review and Planning Meeting 2022-11-08
Udo v. Toussaint

MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

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Status-Report 2022-11-08 : SDTrimSP

Udo v. Toussaint

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SDTrimSP : workhorse for energetic particle-solid interactions (implantation, sputtering, erosion)

- keep code validated, i.e. check discrepancies to other codes

- adapt to fusion specific needs (Tokamak/Stellarator environment)

- consider enhancements relevant/important to ion-solid interaction ↔ data source

- scalability towards DEMO-applications : code or surrogate

RAVETIME : Advection-Diffusion-Reaction code for trap-diffusion dominated H-transport

- include relevant multi-trap-level physics in 3D

- keep code scalable up to very large (i.e. realistic) systems

- verify code (validation ??)

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SDTrimSP : present and ongoing work

- **keep code validated**, i.e. check discrepancies to other codes : SRIM : defect profiles differ

- tracing of differences has been challenging

- specific test case: no vacancies can be created

SDTrim-6.05, W -> W 75 eV; Ed=38 eV, interior start

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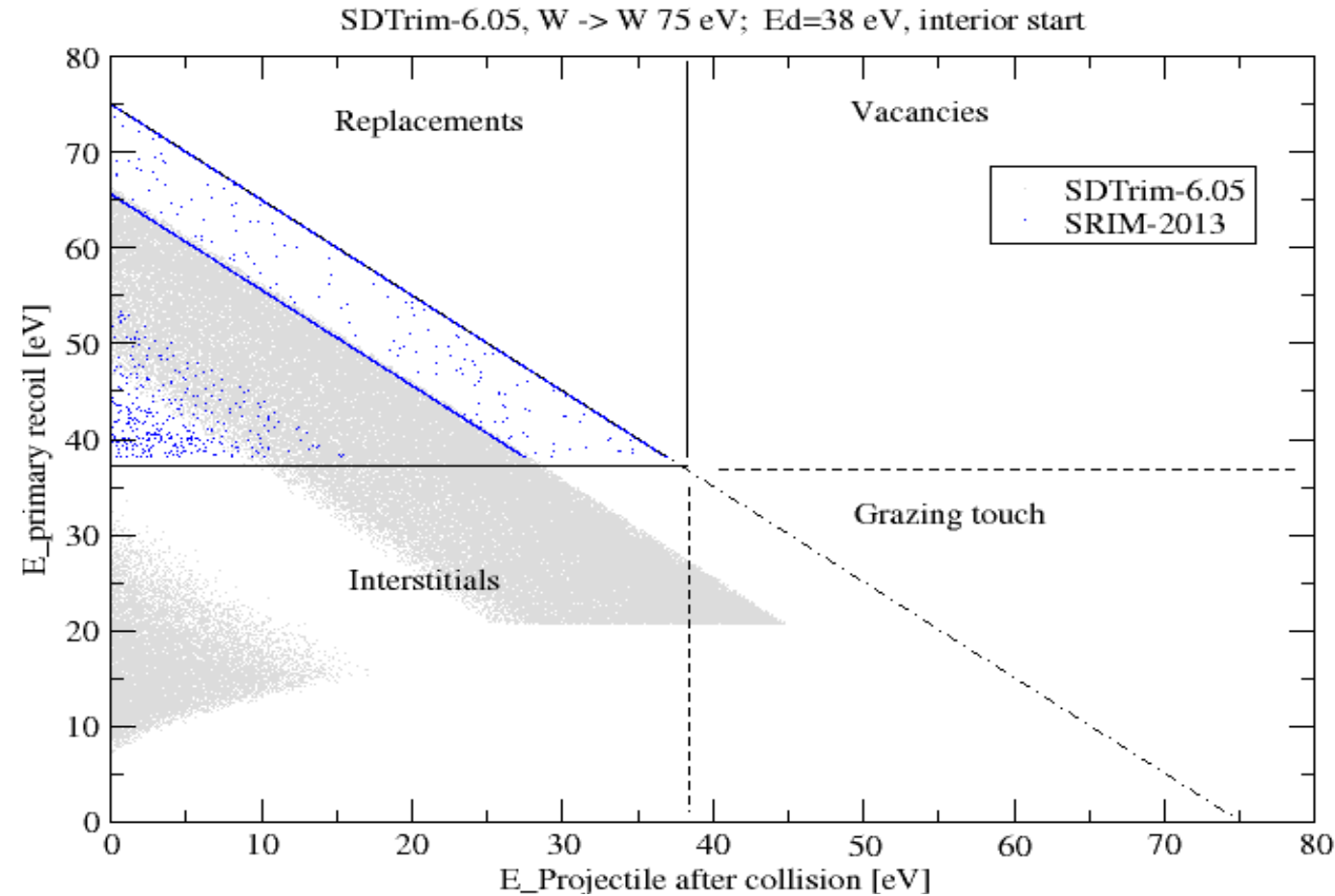
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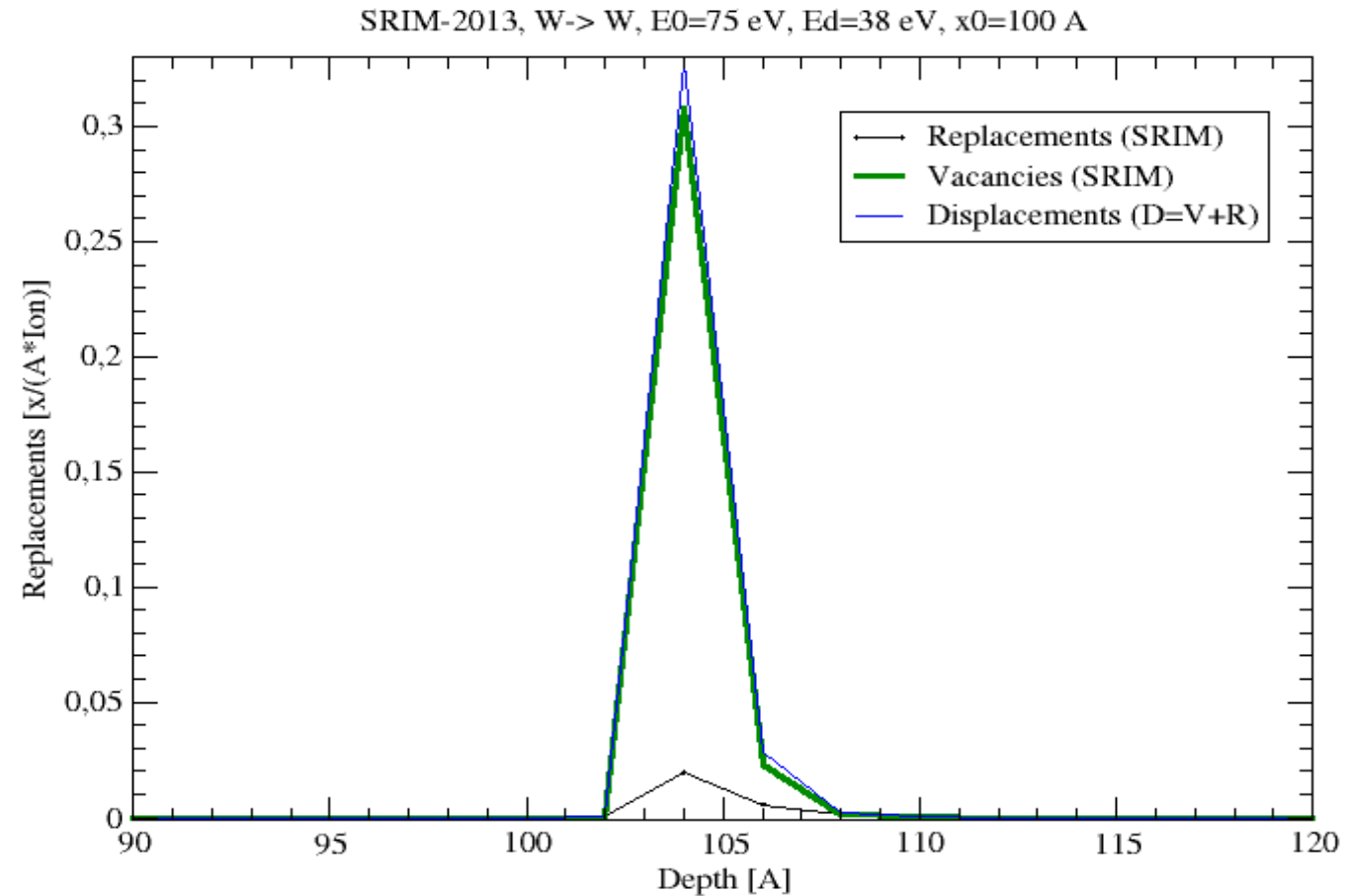
- specific test case: no vacancies can be created

→ SRIM output on vacancies is wrong

→ no known problems for SDTrimSP

SRIM-2013, W-> W, E0=75 eV, Ed=38 eV, x0=100 A

Legend:
- Replacements (SRIM)
- Vacancies (SRIM)
- Displacements (D=V+R)

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- keep code validated, i.e. check discrepancies to other codes : **DONE**

- adapt to fusion specific needs:

    Gyromodul : include magnetic and electric field effects into trajectories (impact angle, ionisation)

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SDTrimSP : present and ongoing work

- keep code validated, i.e. check discrepancies to other codes : **DONE**

- **adapt to fusion specific needs:**

    Optimisation of gyromodul (2022-06):

        - at present for some cases too long run times

            - e.g. late re-ionisation and large gyroradius

            - unequal load balancing in dynamic case

      - coming next:

        - Verification

        - Validation: Evaluation of sample exposure experiments of present AUG campaign

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            - unequal load balancing in dynamic case : **minimized :-)**
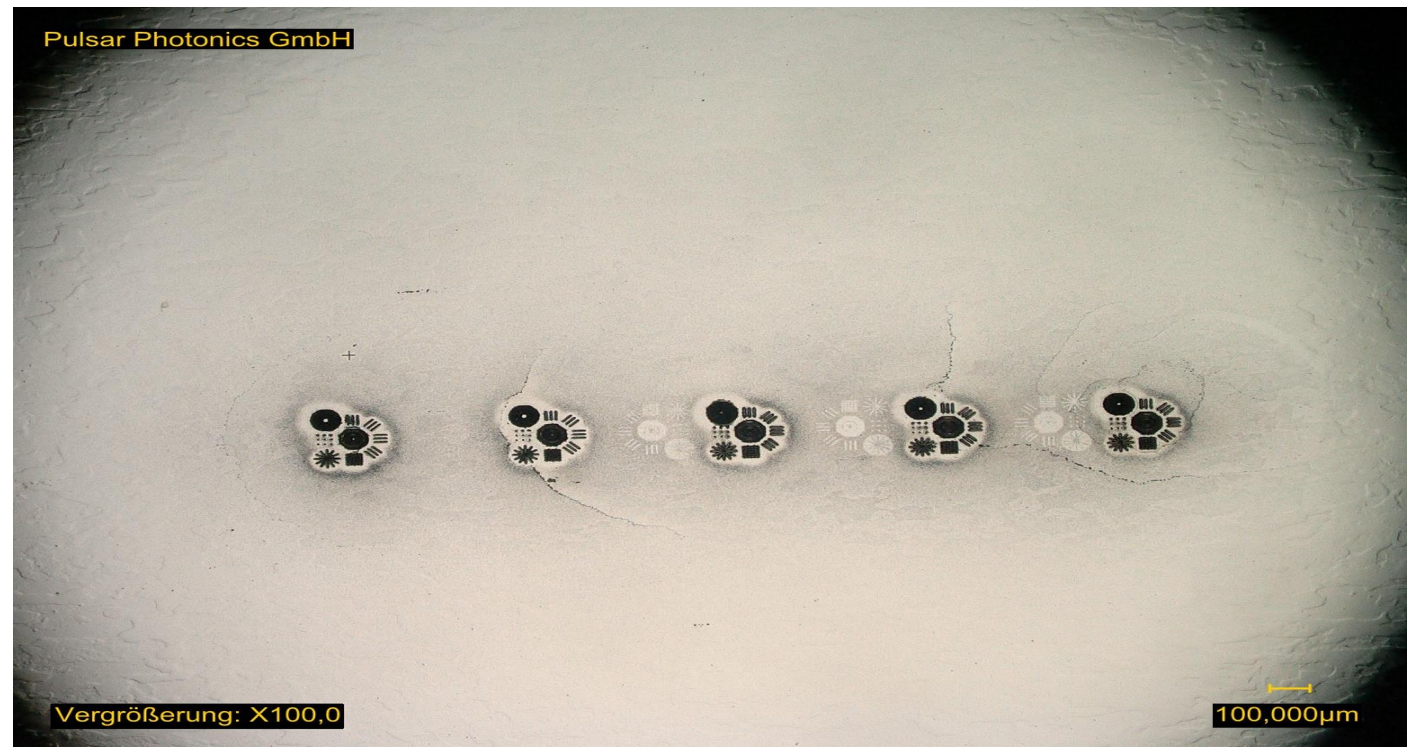
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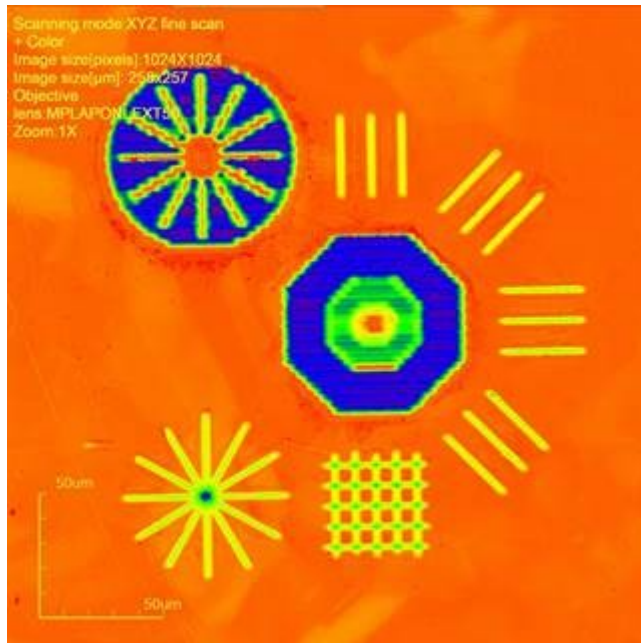
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SDTrimSP : present and ongoing work

- Validation: Evaluation of sample exposure experiments of present AUG campaign

  - Design, manufactoring and analysis of sample with dedicated surface structure

  - Laser structuring process

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SDTrimSP : present and ongoing work

- Validation: Evaluation of sample exposure experiments of present AUG campaign (Summer 2022)

  - Design, manufactoring and analysis of sample with dedicated surface structure (R.Arredondo & M.Balden)
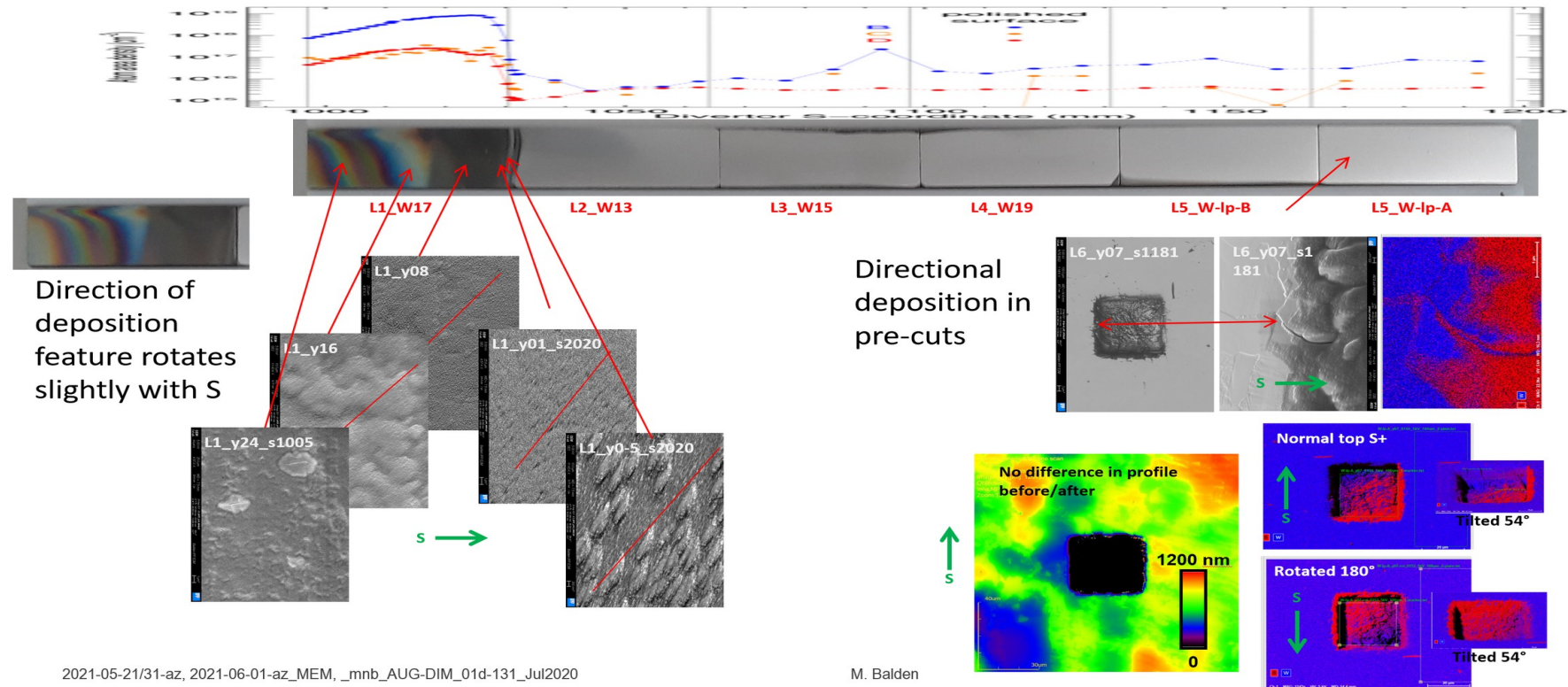
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SDTrimSP : present and ongoing work

- Validation: Evaluation of sample exposure experiments of present AUG campaign (Summer 2022)

   - Design, manufactoring and analysis of sample with dedicated surface structure (R.Arredondo & M.Balden)

   - Laser structuring process: looked promising, but did **not work** on mirror polished W samples :-(
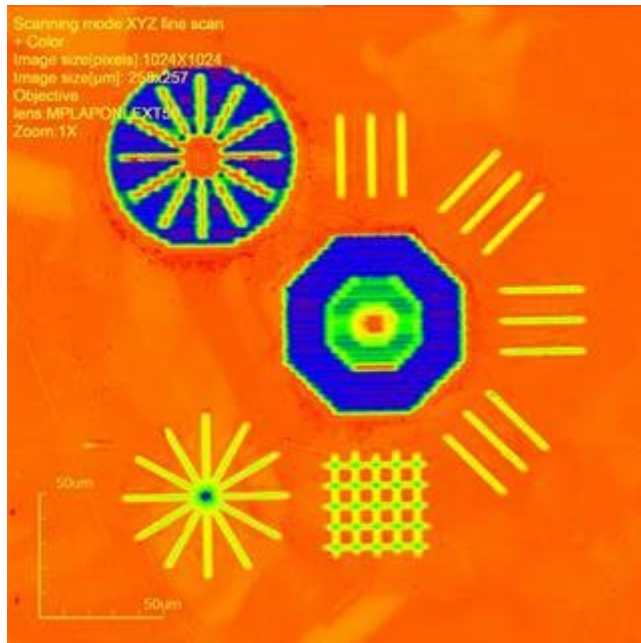
SDTrim-Gyro

- 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… (plasma background, B-orientation)

2021-05-21/31-az, 2021-06-01-az_MEM, _mnb_AUG-DIM_01d-131_Jul2020

M. Balden

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- Consider enhancements relevant/important to ion-solid interaction:

    Going beyond amorphous sample description

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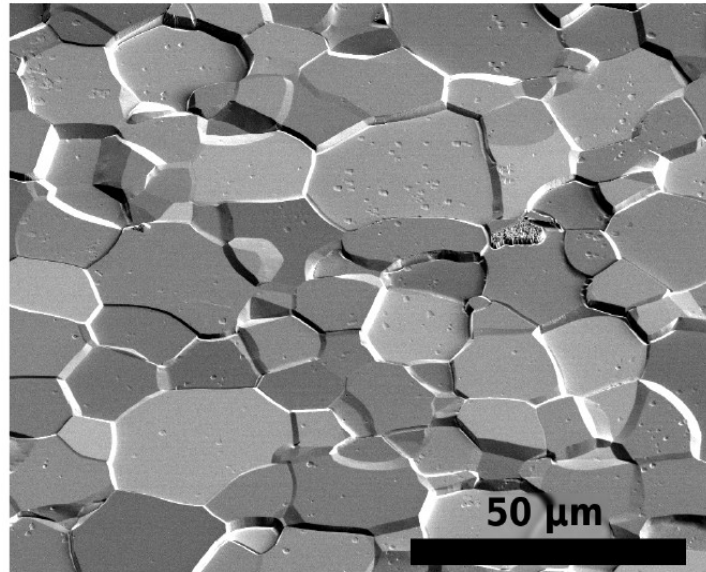- Going beyond amorphous sample description

        - implementation of crystal lattice capabilities: foreseen for next production release
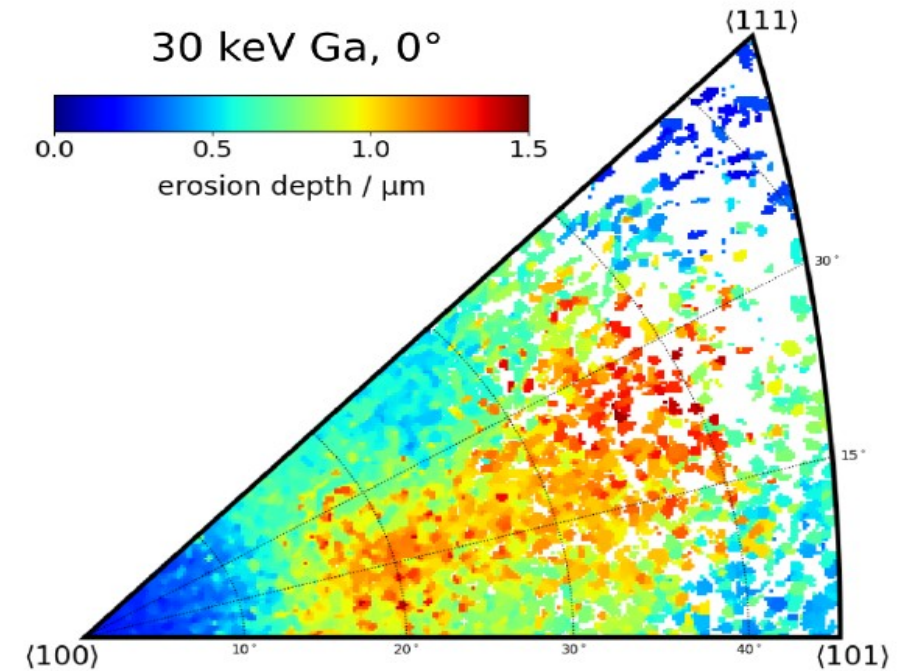
        - cross-validation with MARLOWE and MD

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SDTrimSP : present and ongoing work

- Sputtering can depend on local atomistic structure

images from PhD thesis Karsten Schlüter (2021)

- Available simulation tools are limited : MD, MARLOWE, ...

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SDTrimSP : present and ongoing work

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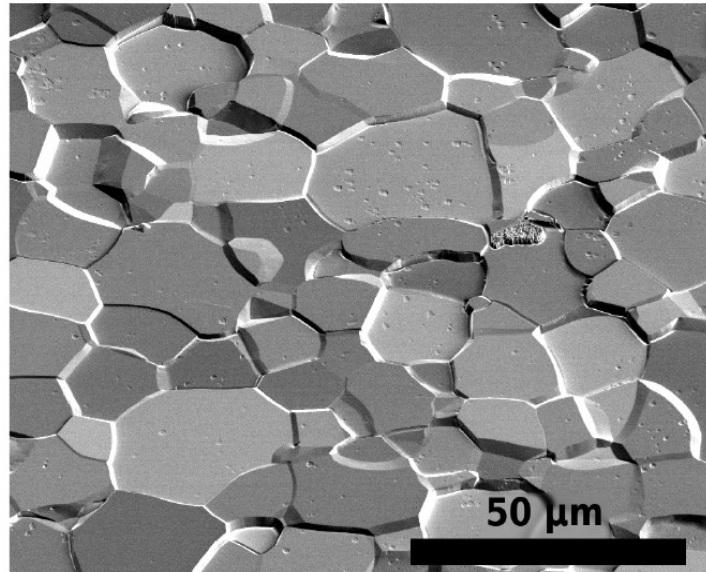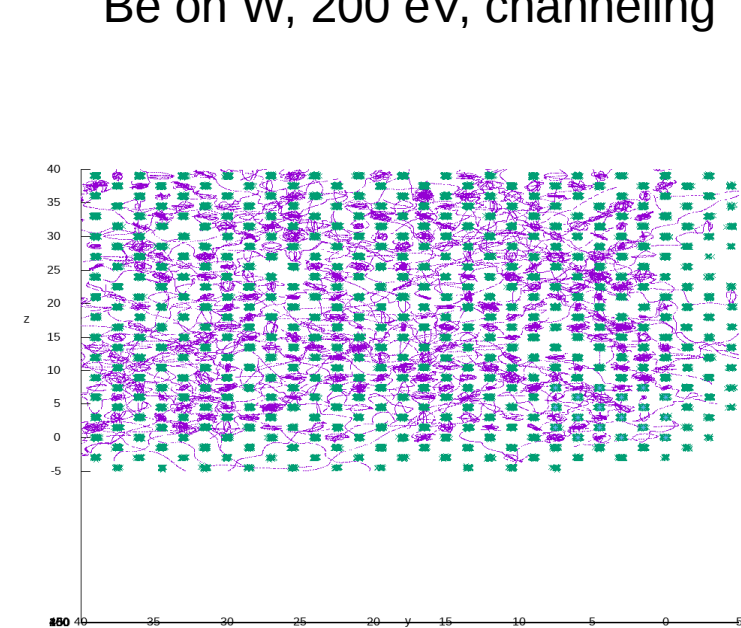

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Be on W, 200 eV, channeling

- Implementation of local lattice structure and/or partial amorphous states into SDTrimSP

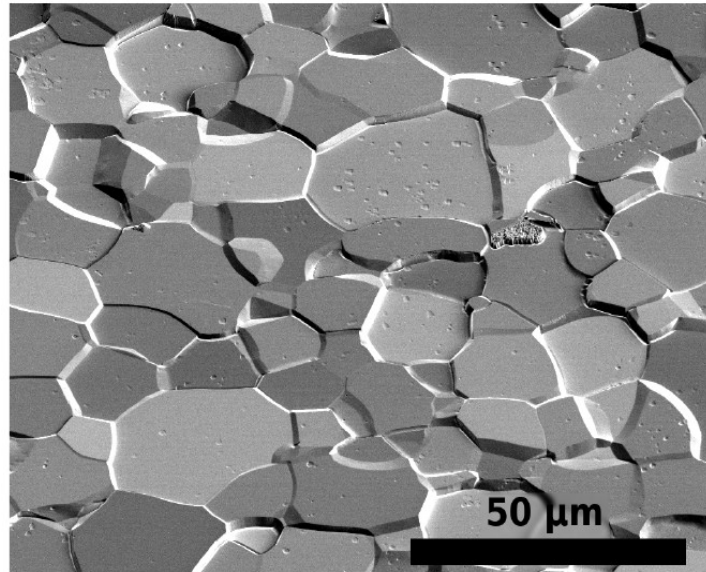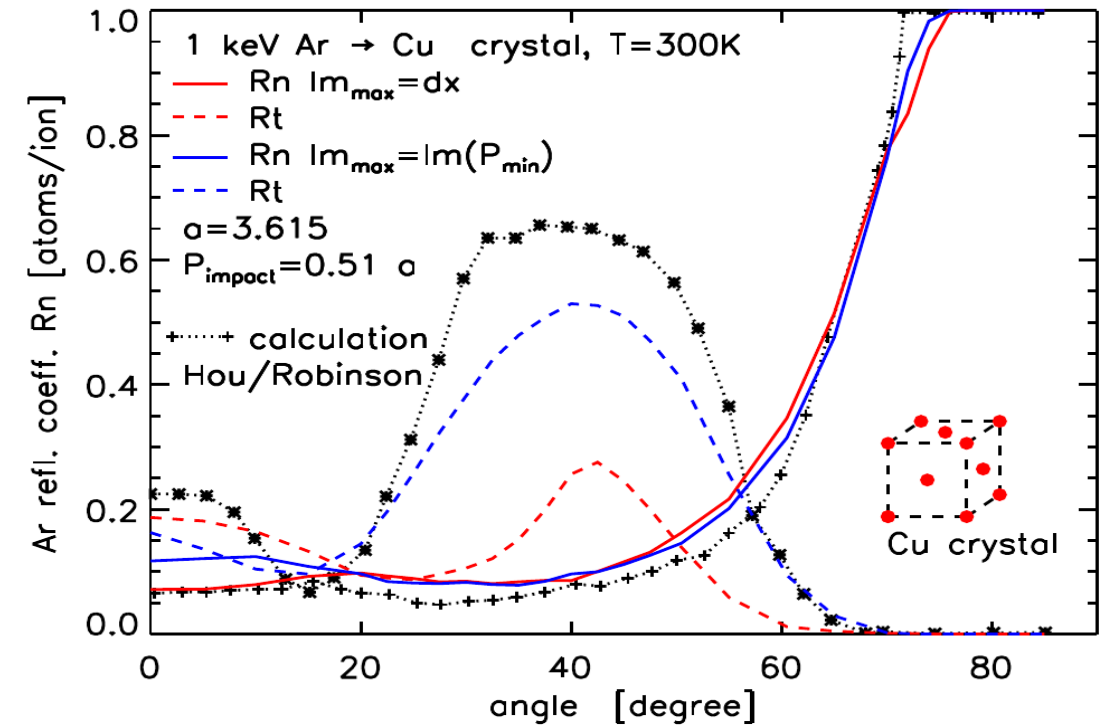## SDTrimSP : present and ongoing work

- Sputtering can depend on local atomistic structure

images from PhD thesis Karsten Schlüter (2021)

- Comparison of SDTrimSP on fcc-lattice structure with MARLOWE (M. Hou et al, NIM 132 p. 641)

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- Going beyond amorphous sample description

        - implementation of crystal lattice capabilities: foreseen for next production release: **on track**

        - next step is cross-validation with MARLOWE and MD: **on track**

Thank you very much!

Questions?

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RAVETIME : present and ongoing work

- Semi-analytical polynomial solver:

    - at low temperatures the equilibrium trap-occupation becomes close to non-differentiable

        - usual root-finding algorithms sometimes converge to wrong solution

        - Test of homotopy methods are promising : now discussion about Open Source…

        → *does not pay off...*

    - coming next:

        - contact with ACH on >their< needs (hopefully...so far no two-way communication): *Nope*

        - test if symplectic methods for the PDE-system offer overall benefits : *refocus on positivity*

        - check if more flexible (and or adaptive) lattice generator desirable/useful ?