EUROfusion

ENABLING RESEARCH PROJECT ENR-MAT.01.VR

Electronic interactions of slow ions and their influence on defect formation & sputter yields for plasma facing components

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EUROfusion Science Meeting on Status of Enabling Research Projects, 28th of September 2022

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Outline

- Aim;
- Working-packages & team;
- Main results obtained & work in progress;
- Achievement of Scientific Deliverables foreseen for 2022;
- Activities foreseen for 2023.

Aim

- To investigate underlying quantities fundamental for sputtering and defect formation from plasma-wall interaction:
  →Energy deposition of plasma species in wall materials.
  →Interaction potentials with wall species.

key input variables for computer codes used to model erosion and implantation in plasma facing components.

Synergistic study:

- Experimental measurements with high accuracy.
- Theoretical calculation from first principles.
- To assess the sensitivity of these quantities to the presence of defects (ion irradiation).
- Benchmark the fundamental quantities by measuring sputtering yields with high accuracy.

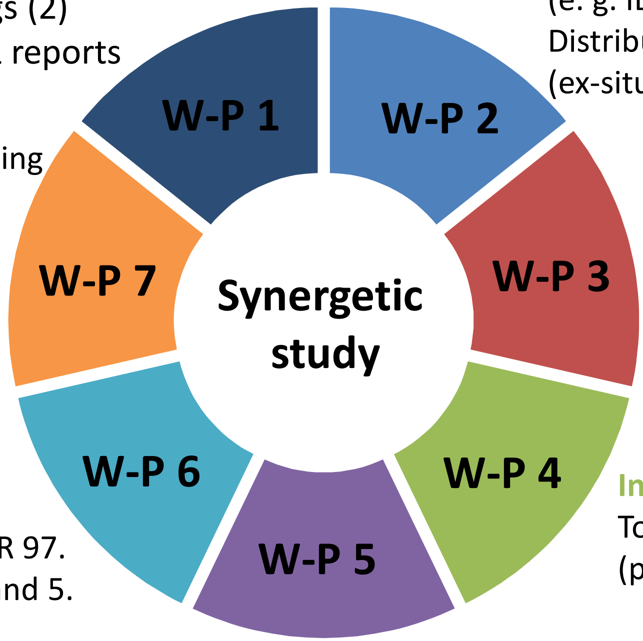
- **Materials:**
  →ITER-grade W, Fe and EUROFER steel.

Working-packages

General management
Kick-off meeting
Task coordination
Annual meetings (2)
Final meeting & reports

Sample preparation
Batches of Fe, W, and EUROFER97.
Chemical and morphological characterization (e. g. IBA; AFM; XRD).
Distribution and routinely quality control (ex-situ and in-situ).

Computational modelling
TDDFT simulations of electronic stopping power of W, Fe, and EUROFER-like (with/without defects).
MDRANGE: ion implantation & Sputter yields (Input: electronic stopping)



Electronic energy loss measurements
Experimental stopping cross-section of pristine Fe, W, and EUROFER97.
Energy range: sub-keV to MeV.
Compare experimental results between pristine & damaged.

Ion-irradiation experiments
Ex-situ and In-situ ion irradiation experiments on Fe, W, and EUROFER 97.
Samples to be reused in W-Ps 3,4, and 5.

Interatomic potential measurements
ToF-LEIS & ToF-MEIS angular scans measurements (pristine and damaged samples).

Sputtering yield & QCM
QCM set-up at UU. Sputtering yield and angular distribution of pristine Fe, W, and EUROFER 97 samples. BCA-based simulations (SDTrimSP).

Team

VR	ÖAW	VTT
Eduardo Pitthan (PI)	Christian Cupak	Andrea Sand
Jila Shams-Latifi	Martina Fellinger	Ludovico Caveglia Curtil
Petter Ström	Friedrich Aumayr	Tetiana Malykhina
Per Petersson		

Start: May of 2021.

VR main tasks: Sample preparation and characterization, electronic loss measurements, interatomic potential measurements, and ion irradiation experiments.

ÖAW main tasks: Sputtering yield measurements, and BCA-based simulations.

VTT main tasks: Computational modelling (simulations of electronic stopping power & ion implantation).

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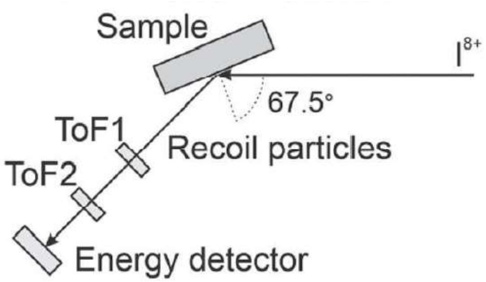
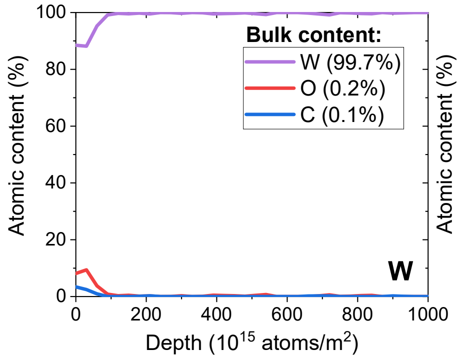
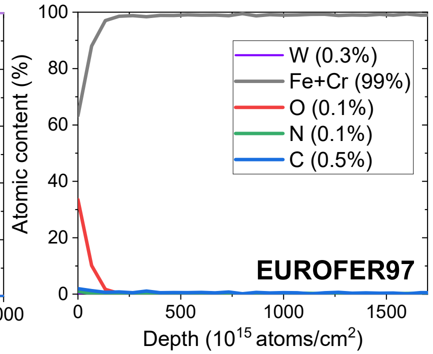
W-P 2: Sample preparation

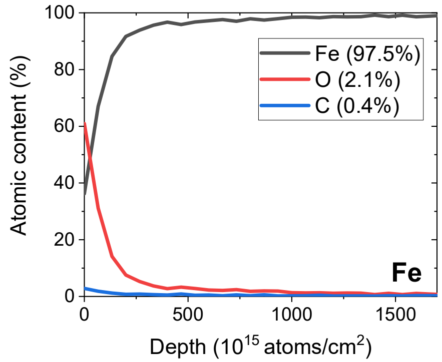
Characterization of the chemical composition of the pristine samples (Fe, W, EUROFER) by combined ion beam based techniques (UU), as a protocol for the standard quality control.

→Atomic concentration depth profiles by ToF-ERDA:



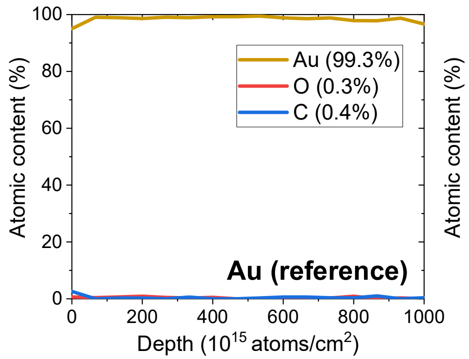


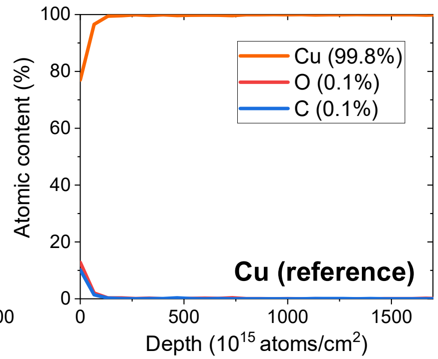




→Low impurity concentrations in bulk.

Evaluation window 500-1000×10^{15} atoms/cm^2





Final stopping data corrected by Bragg's rule:

$$\epsilon^{A_m B_n \cdots} = m\epsilon^{A} + n\epsilon^{B} + \cdots$$

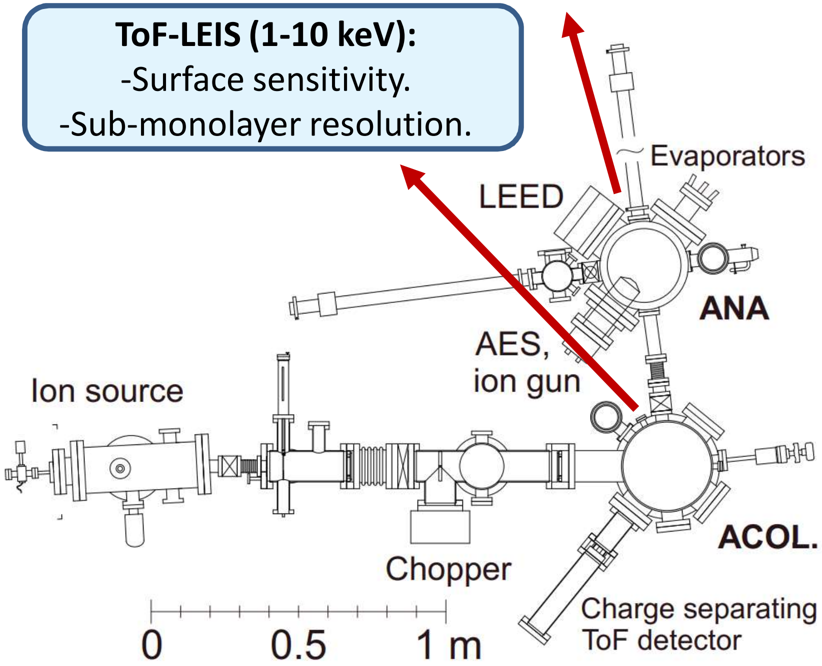
W-P 3: Electronic energy loss measurements

Experimental procedure for low energy regime

ACOLISSA experimental set-up:

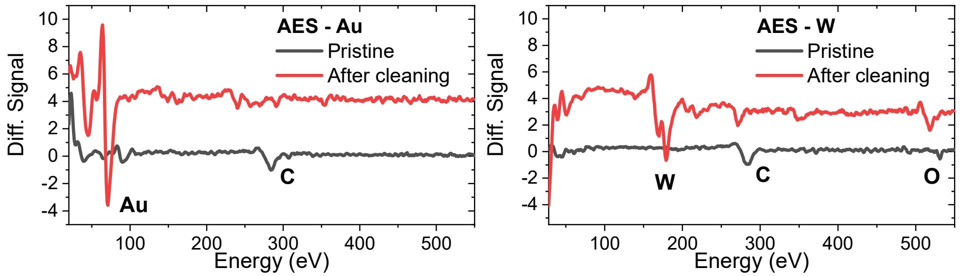
Analytical Chamber: Sputtering cleaning, annealing, AES, e⁻beam evaporation, and LEED.

ToF-LEIS (1-10 keV):
-Surface sensitivity.
-Sub-monolayer resolution.

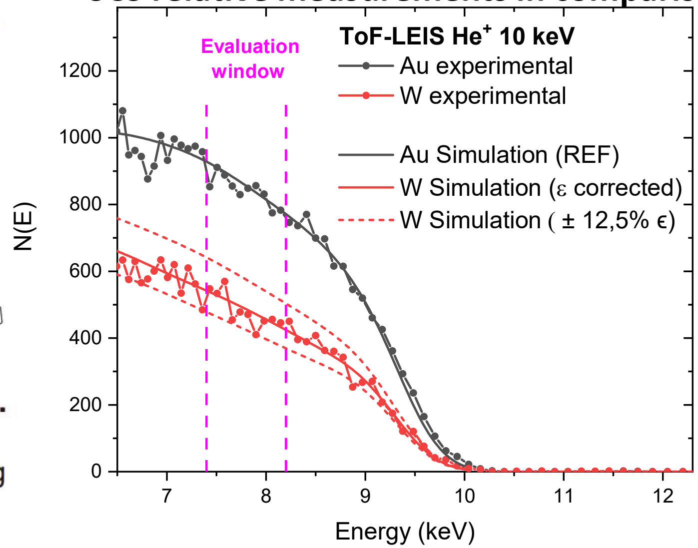


P. Ström and D. Primetzhofer 2022 JINST 17 P04011

***Sample cleaning:** cycles of Ar^+ sputtering 3 keV 30˚.*



SCS relative measurements in comparison with MC simulations:



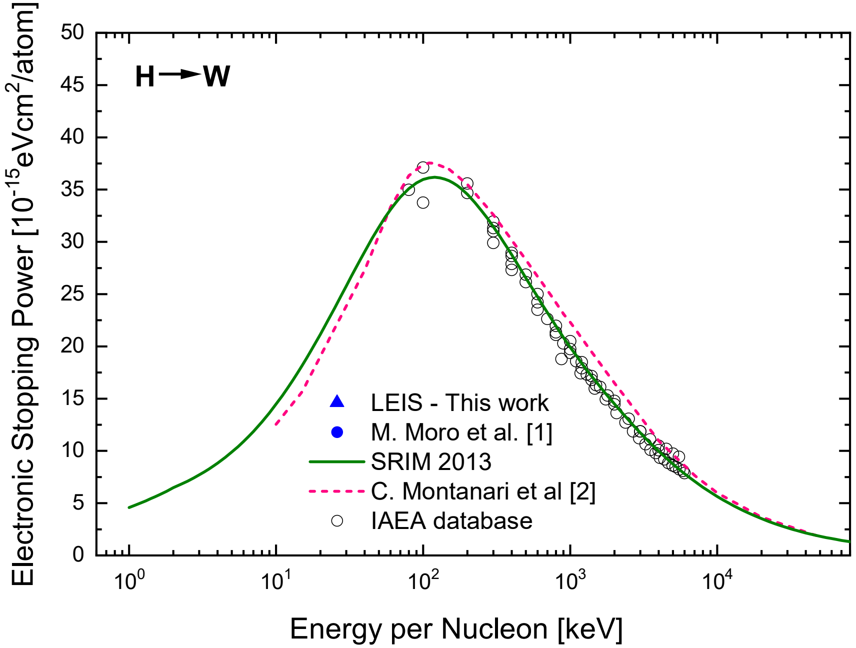
→Cu/Au as reference under same experimental condition.

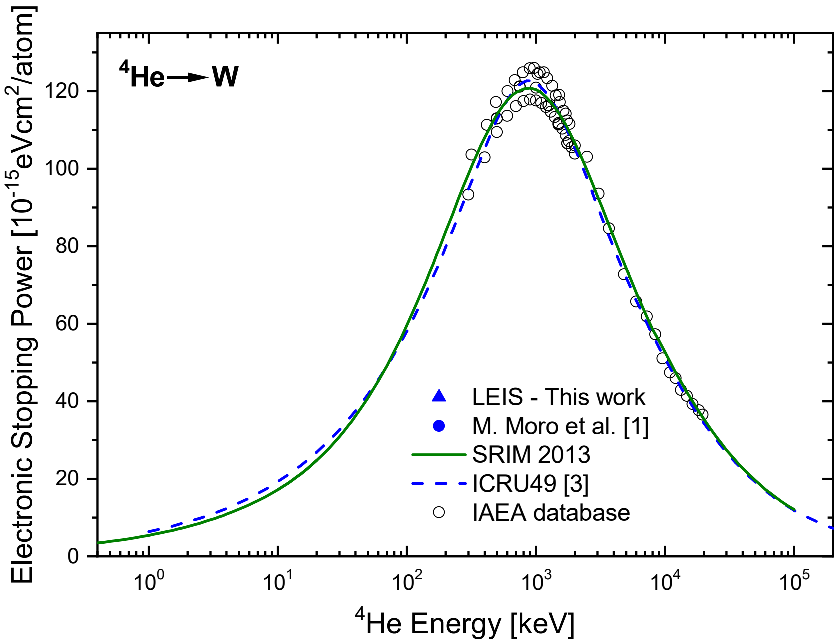
→SCS extraction from height ratio.

→ Similar approach for MEIS and MeV energies our laboratory.

W-P 3: Electronic energy loss measurements

Experimental stopping cross-section of pristine Fe, W, and EUROFER97

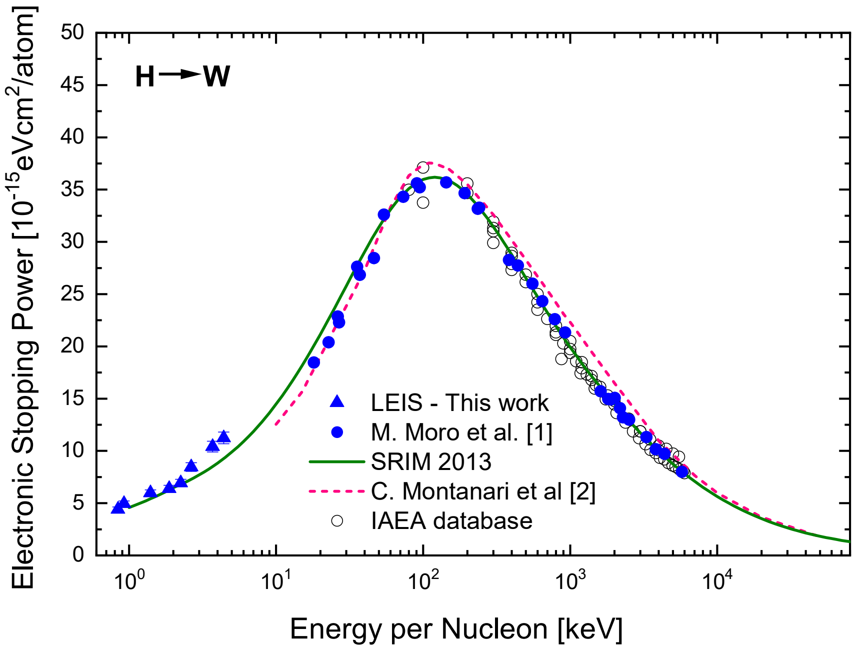


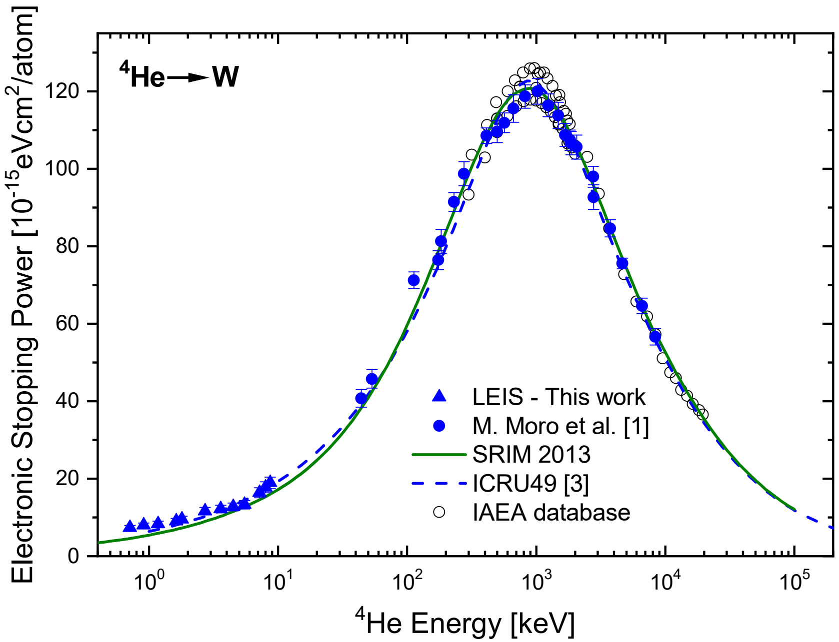


[1] M. V. Moro et al., Nucl. Instrum. Meth B **498** (2021).
[2] C. C. Montanari et al., Phys. Rev. A **80**, 012901 (2009).
[3] M. J. Berger, et al., Report 49, Oxford Academic (1993).

W-P 3: Electronic energy loss measurements

Experimental stopping cross-section of pristine Fe, W, and EUROFER97



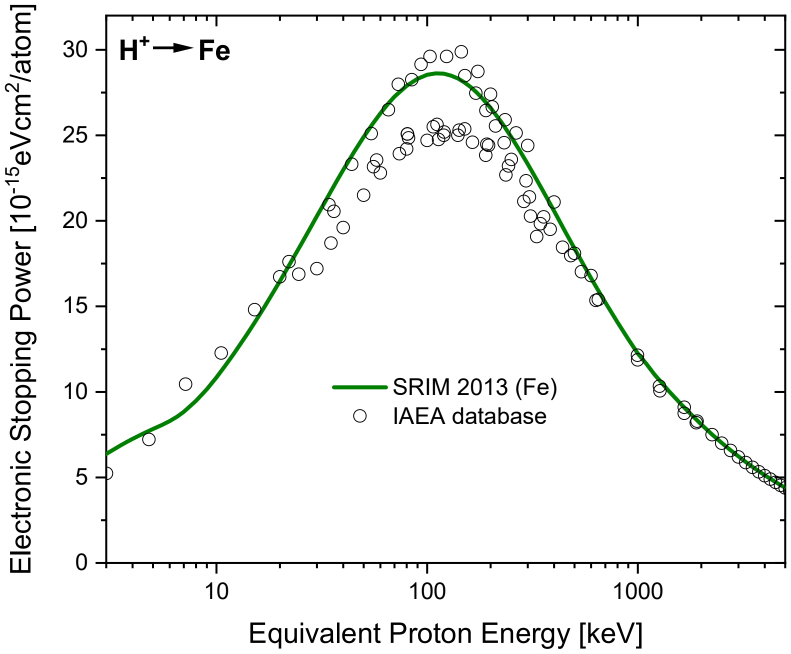


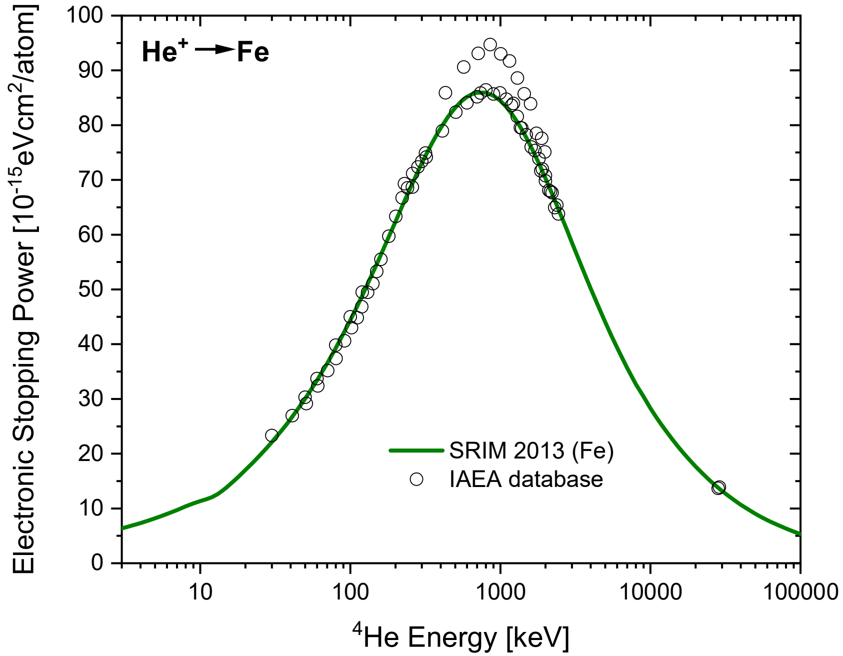
MEIS and MeV Range [1]: Good agreement with experimental and SRIM 2013 (up to 3.5% for protons and 4.0% for He).
LEIS: Discrepancies from SRIM-2013 up to 20% for protons and 60% for He (good agreement with ICRU49).

[1] M. V. Moro et al., Nucl. Instrum. Meth B **498** (2021).
[2] C. C. Montanari et al., Phys. Rev. A **80**, 012901 (2009).
[3] M. J. Berger, et al., Report 49, Oxford Academic (1993).

W-P 3: Electronic energy loss measurements

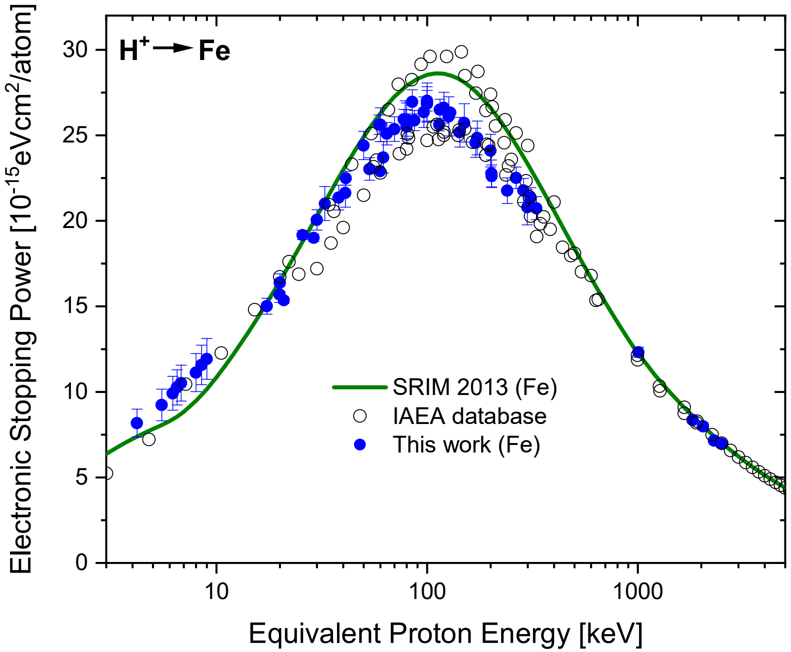
Experimental stopping cross-section of pristine Fe, W, and EUROFER97

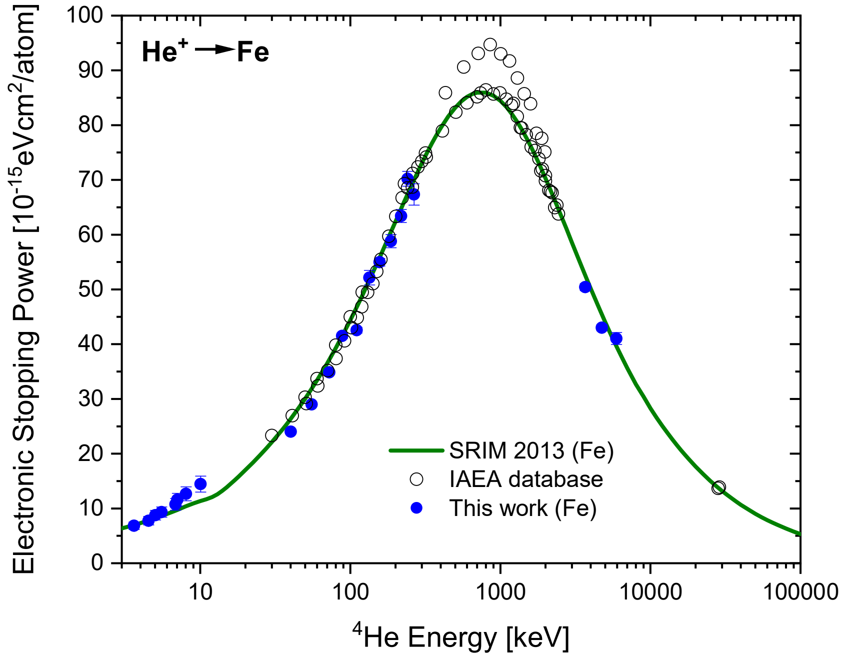




W-P 3: Electronic energy loss measurements

Experimental stopping cross-section of pristine Fe, W, and EUROFER97





H^+ → Fe

→ Good agreement at MeV range.

→ Large discrepancy with SRIM around maximum (up to 11%).

→ Large discrepancy with SRIM at low energy range (up to 20%).

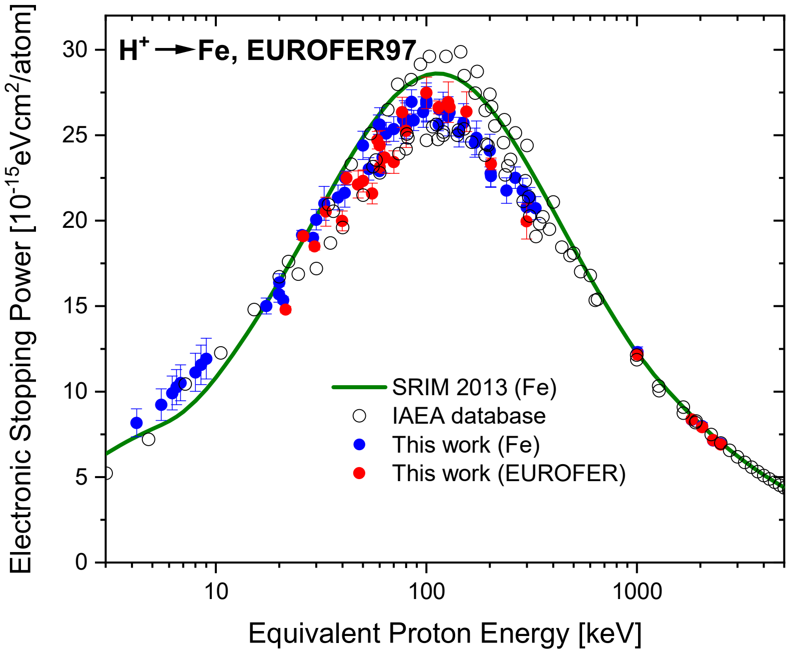
He^+ → Fe

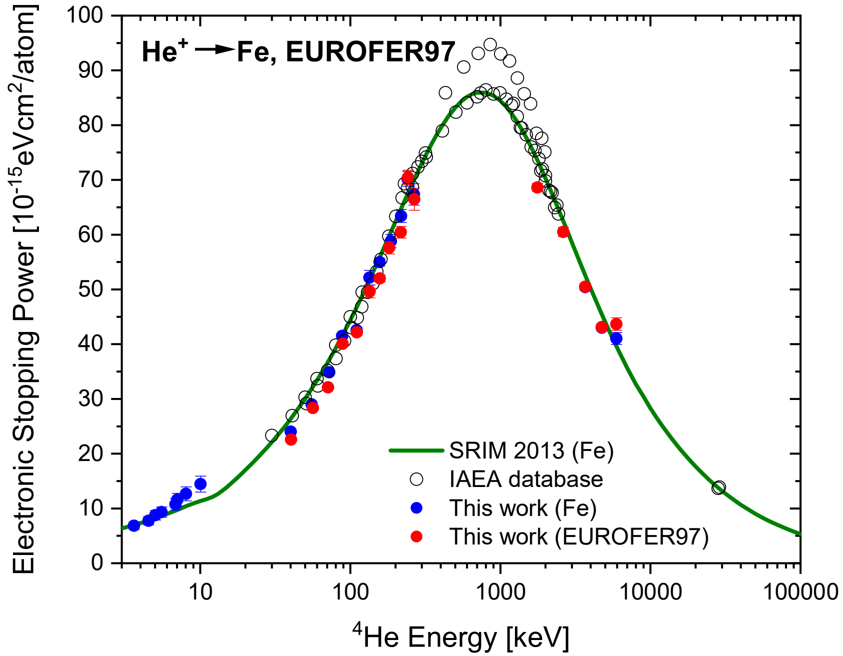
→ Good agreement at keV/MeV range within 6%.

→ LEIS: discrepancy up to 26%.

W-P 3: Electronic energy loss measurements

Experimental stopping cross-section of pristine Fe, W, and EUROFER97





H^+, He^+ → EUROFER97

→ EUROFER97: similar SCS to Fe.

→ No clear deviation from Bragg's rule

In progress (this year):

→ EUROFER97 SCS at LEIS (absolute and relative approach).

W-P 4: Interatomic potential measurements

Crystal samples received (March 2022):
W(110), Fe(100), Cr(100)

- **In the LEIS regime (1-10 keV):**
- **Scattering potential (Thomas-Fermi-Molierè):**

$$V(r) = \frac{Z_1 Z_2 e^2}{r} . \Phi(\frac{r}{a})$$

Screening function

Screening lenght

$$a = c_a a_f$$

Screening correction factor (empirical)

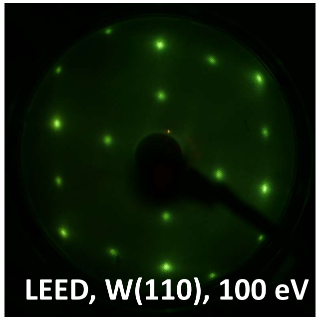
For a given θ:

$c_a < 1$ → smaller scattering cross-section.

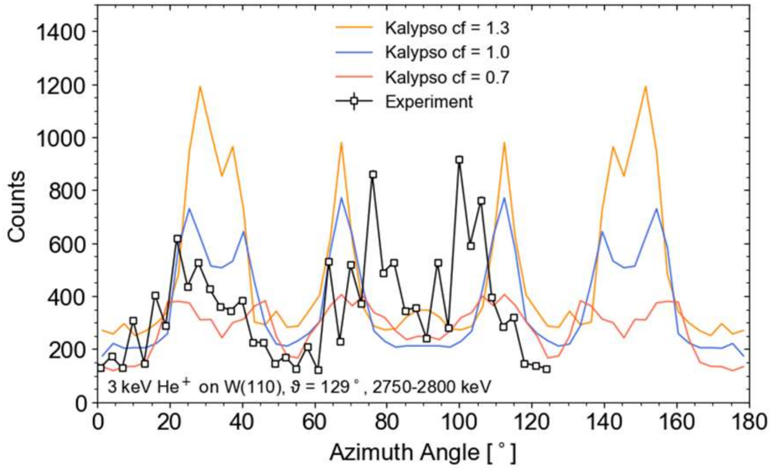
The plan:
Measuring the interatomic potential of W, Cr, and Fe by comparing angular LEIS scans with KALYPSO simulations.

Experiment:

- W(110) sample
- Multiple cycles of sputter cleaning and annealing
- Azimuth scan from 0° to 132° using 3 keV He^+



ToF-LEIS, 3 keV He^+



Experiments and simulations are in progress.

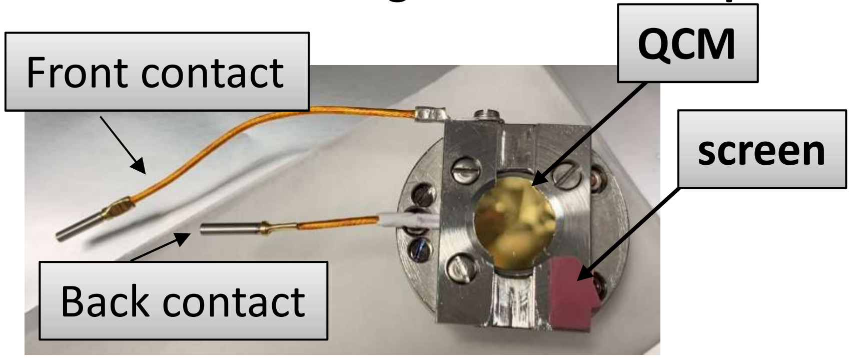
Simulations:

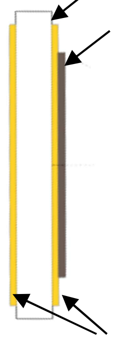
- Using KALYPSO, a software for molecular dynamics simulation of atomic collisions in solids.
- Using Thomas-Fermi-Moliere potential under different corrections.

W-P 5: Sputtering yields and BCA simulation

QCM (Quartz Crystal Microbalance) set-up with low noise and high sensitivity for mass changes (≈ 90 pg/cm²/s). [1,2]

QCM holder designed for UU setup:



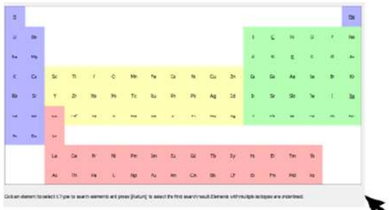


$$-\frac{\Delta f}{f} = \frac{\Delta m}{m}$$ [3]

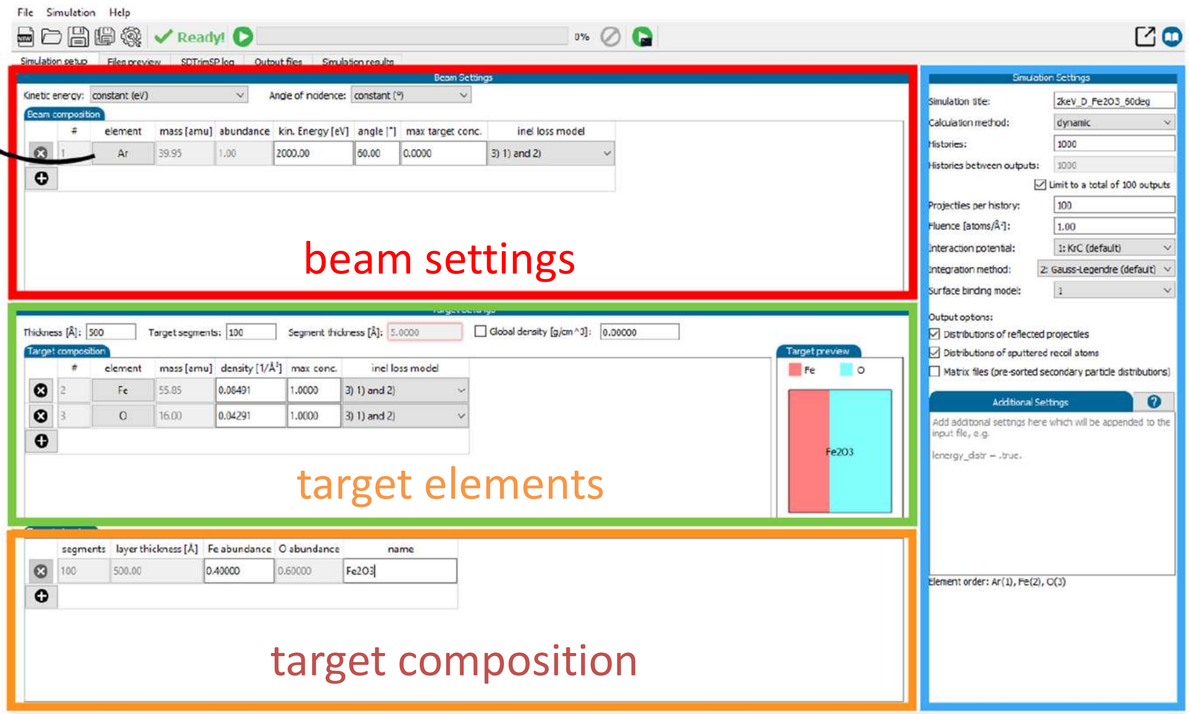
Preparation: At TU Wien, new electronics and hardware components constructed.
Installation: TU Wien campaign by C. Cupak and M. Fellinger (October 2021).
Features: *In-situ* mass-change measurements and subsequent IBA (RBS, ERD).
Tests: Investigation of the formation of photochromic films (33104 at EUROFusion Pinboard).

[1] G. Hayderer et al., Rev. Sci. Instrum. **70**, 3696 (1999)
[2] R. Stadlmayr *et al.* Rev. Sci. Instrum. **91**, 125104 (2020)
[3] G. Sauerbrey, Z. Physik **155,** 206-222 (1959)

W-P 5: Sputtering yields and BCA simulation



Development of a SDTrimSP-GUI



special settings
(dynamics, statistics, potentials, extras)

- easy-use (like SRIM)
- live visualisations
- Quick parameter sweep
- (e.g, potentials, binding energies,…)
- Other BCA codes soon integrated (TRIDYN, IMSIL)

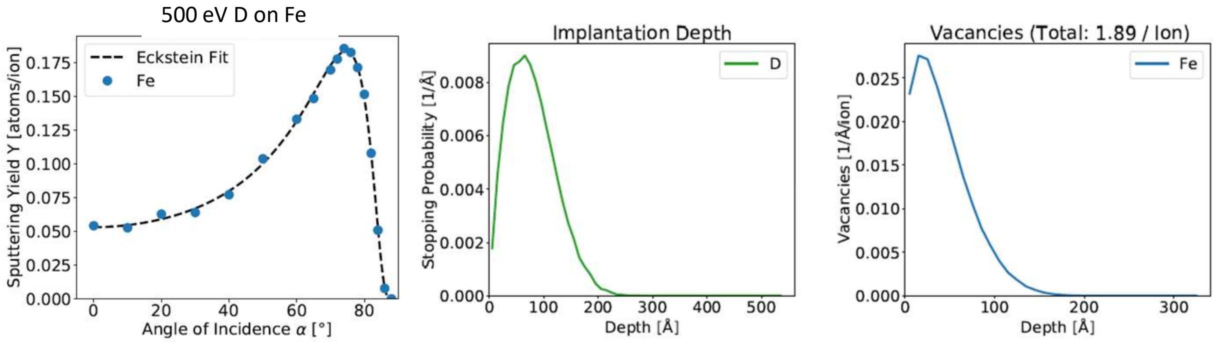
https://doi.org/10.1016/j.nimb.2022.04.008

W-P 5: Sputtering yields and BCA simulation

SDTrimSP-GUI

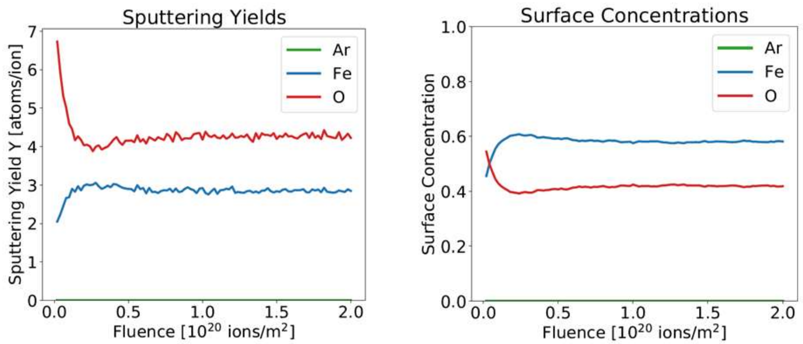
Static calculations:

- Incidence angle sweeps
- Ranges and vacancies
- Particle emission vectors



Dynamic calculations:

- Sputter yields, composition,…



Large benefit for ENR project (parameter tuning,…)

Paper published in NIMB [1]

[1] https://doi.org/10.1016/j.nimb.2022.04.008

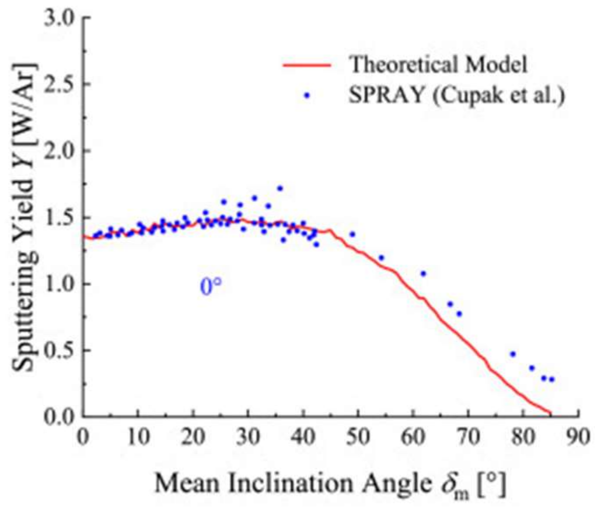
W-P 5: Sputtering yields and BCA simulation

Analytical model for roughness

- nm-roughness can affect sputtering
- Relevant when comparing numerical and experimental results
- Analytical model established to predict sputtering effects for (Gaussian) rough surfaces

- Paper published in Surf. Interfaces [2]

2keV Ar on W, 0° incidence angle



→ can be used to consider effects for our data, based on surface roughness parameter δ_m

[2] https://doi.org/10.1016/j.surfin.2022.101924

W-P 5: Sputtering yields and BCA simulation

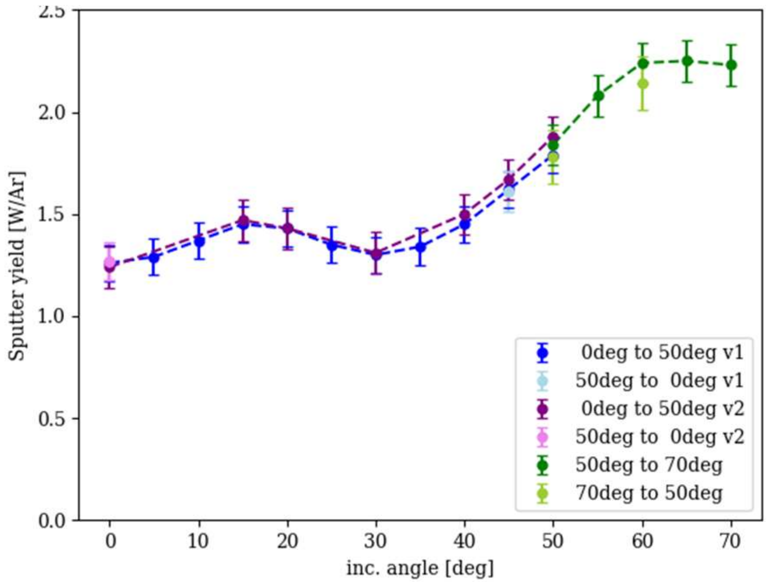
QCM experimental data on W sputtering

- Flat W, sputtered by 2 keV Ar^+
- Local minimum at 30° observed
- Channeling effects in a (poly) crystalline sample suggested
- Also observed for D^+ irradiation
- XRD and EBSD measurements ongoing

Outlook:

- QCM experiments with EUROFER-97
- IMSIL simulations (BCA sputter code with crystallography features)
- MD simulations (A. Sand)

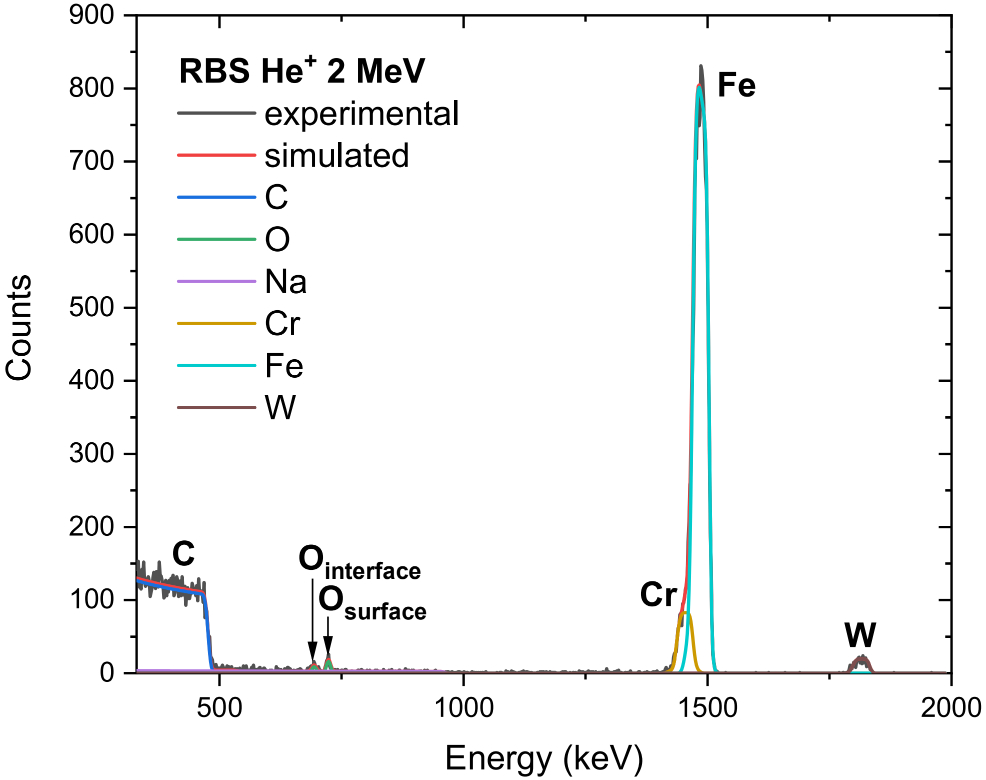
2keV Ar^+ on W



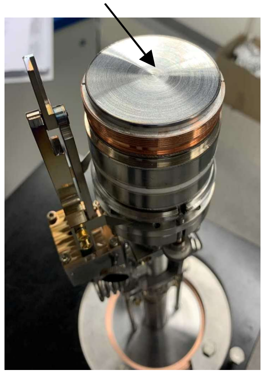
W-P 5: Sputtering yields and BCA simulation

Formation and characterization of thin films from EUROFER97 target

In collaboration with P. Petersson and M. Rubel [1]



Sputtering target (2 inches):



Sputtering conditions:

P_{base} = 7.1×10^{-8} mbar

P_{Ar} = 5.61×10^{-3} mbar

f_{Ar} = 10 sccm

P = 25 W

$Rate_{QCM}$ = 4.91 nm/min

From SIMNRA: Similar composition to bulk.

	At. content (%)	
	Sputtering	Bulk (nominal)
Fe	88.7	88.9
Cr	11.0	9.5
W	0.3	0.3

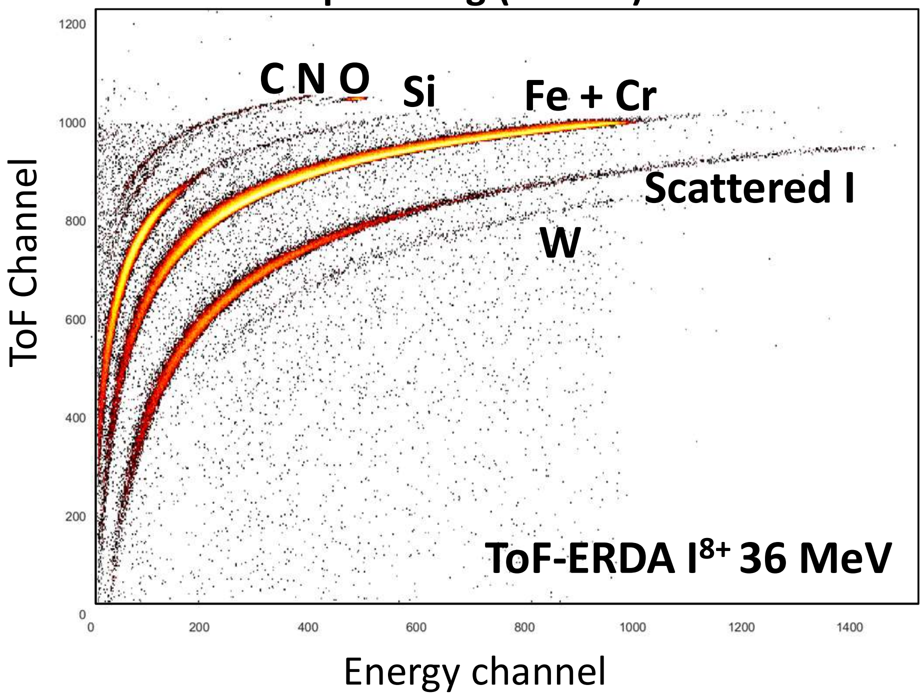
[1] KTH Royal Institute of Technology, Stockholm, Sweden

W-P 5: Sputtering yields and BCA simulation

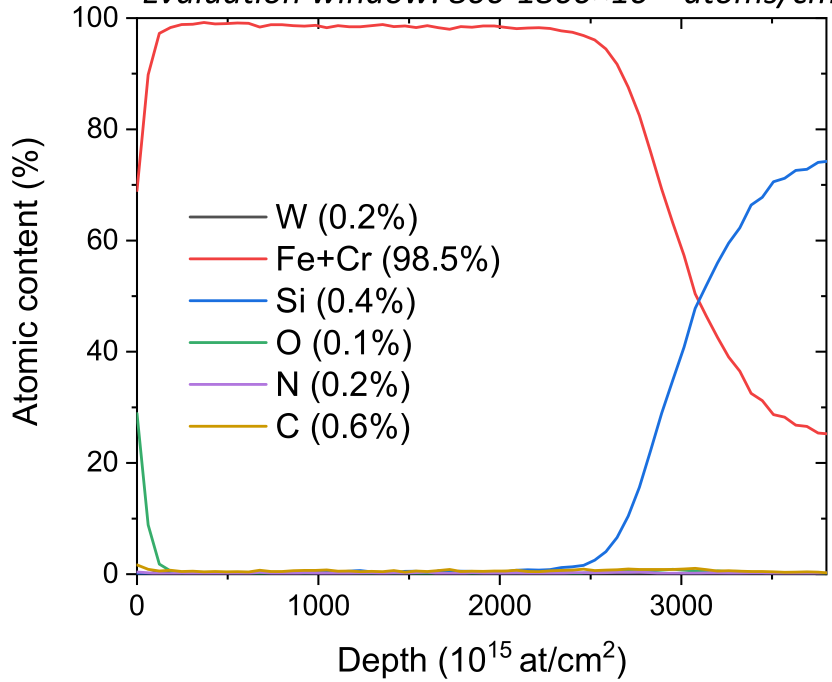
Formation and characterization of thin films from EUROFER97 target

In collaboration with P. Petersson and M. Rubel [1]

EUROFER97 Sputtering (60 min) on Si substrate



Evaluation window: 800-1800×10^15 atoms/cm^2



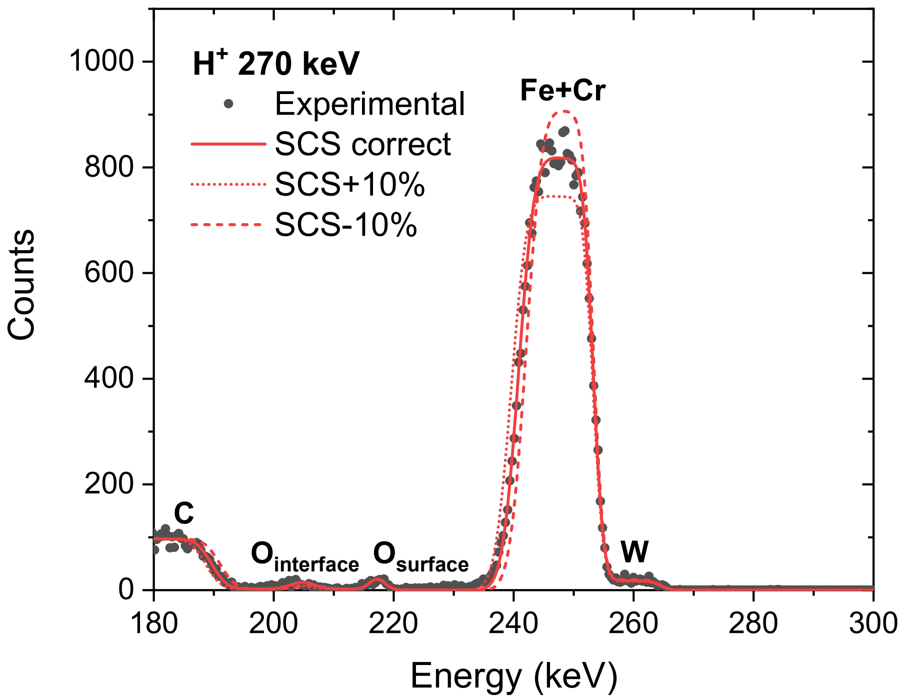
→ Homogeneous with low presence of contaminations.

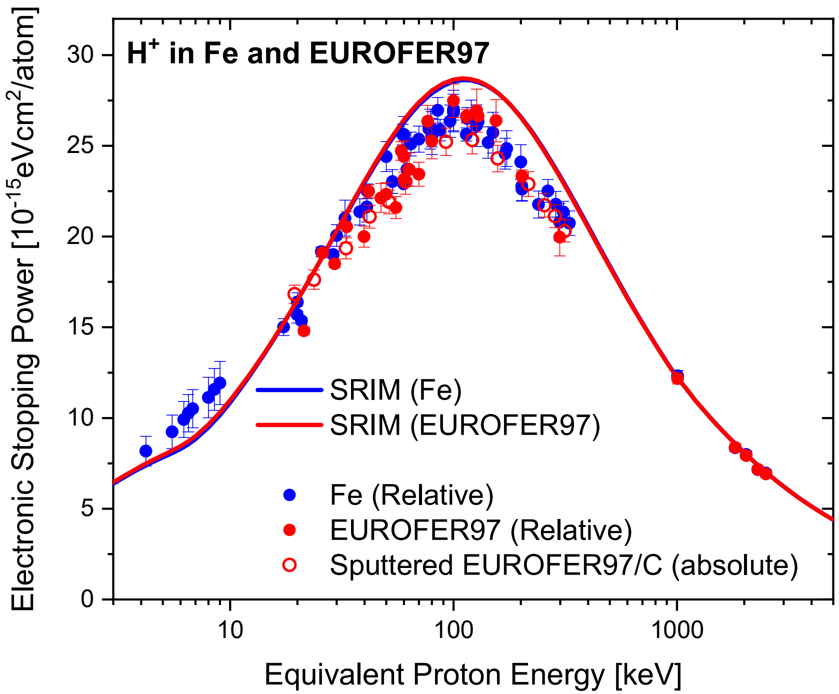
[1] KTH Royal Institute of Technology, Stockholm, Sweden

W-P 3: Electronic energy loss measurements

Electronic SCS of thin films from EUROFER97 target

→ SCS based on the width of spectra in comparison to SIMNRA simulations (absolute approach).





→ Similar behaviour in comparison to relative approach (within 5%).

→ Similar SCS trend between bulk and redeposited EUROFER97.

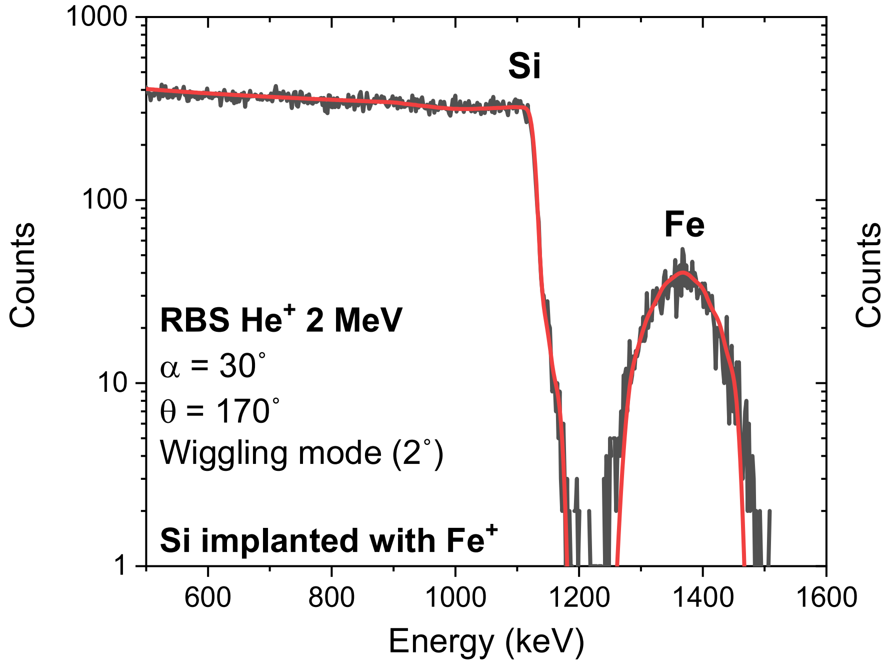
W-P 6: Ion-irradiation experiments

self-irradiation → *High levels of displacement damage without impurities.*

Ion Energy → *High levels of displacement damage within depth from SCS evaluation window.*

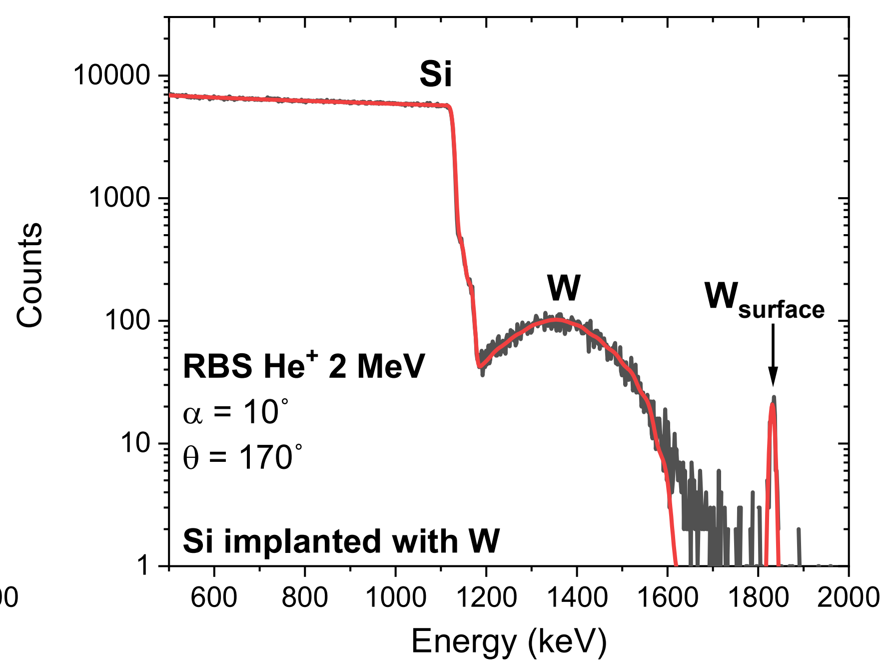
Fe^{+} 300 keV → Fe, EUROFER, Si samples

Fe areal density: 42.25×10^{15} Fe/cm^2



W^{2+} 2.84 MeV → W and Si samples

W areal density: 1.57×10^{15} W/cm^2



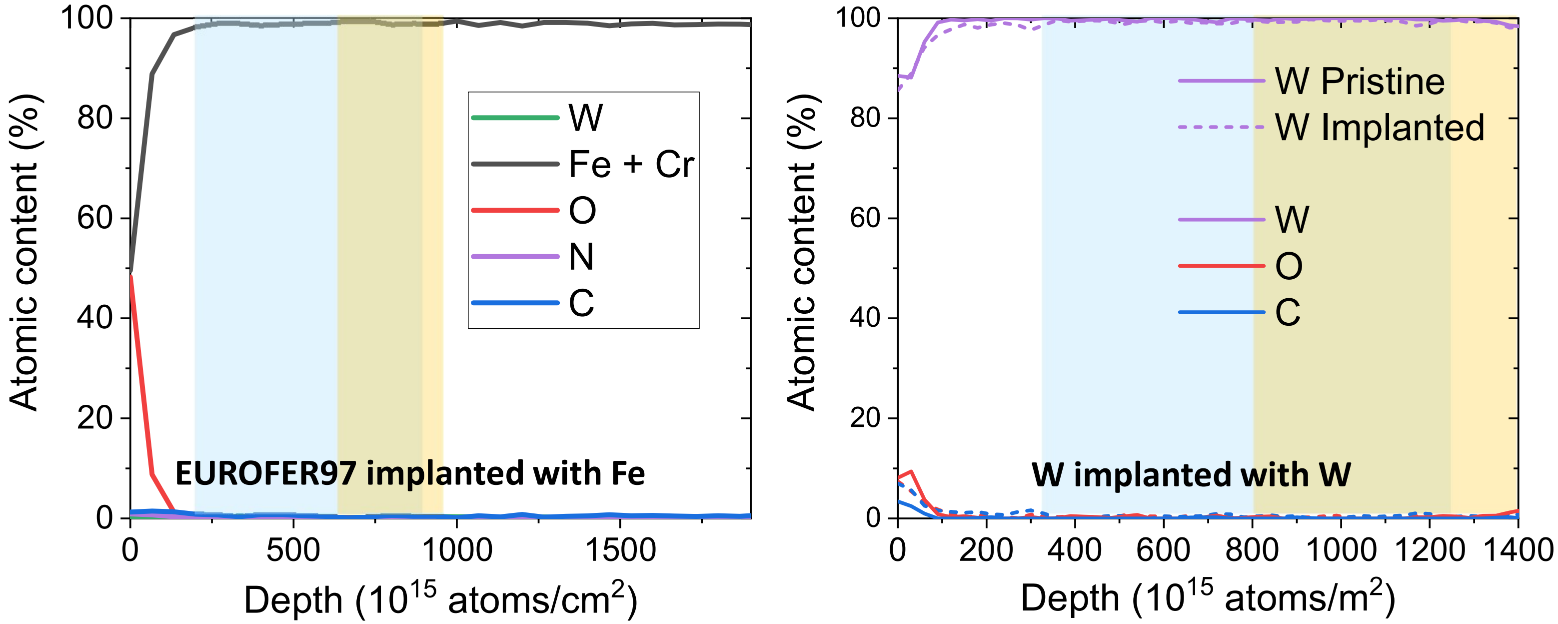
W-P 6: Ion-irradiation experiments

TRIM simulation:

→ Maximum damaged region

→ Ion range

ToF-ERDA (I^{8+} 36 MeV):



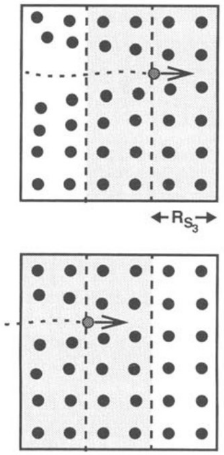
No significant modification on composition on self-irradiated samples.

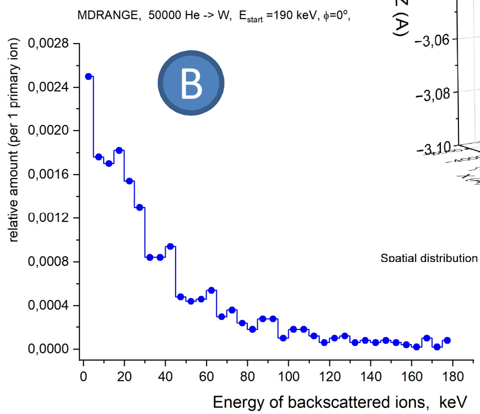
W-P 7: Computational modelling

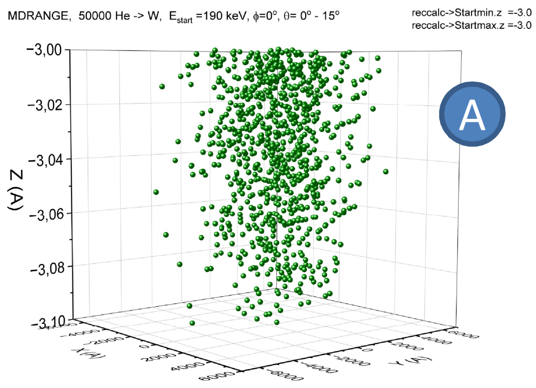
Ion backscattering with MDRANGE (D7.3)

- Principle of MDRANGE: efficient ion range calculations by considering only small region of target in MD framework
- Explicit atomic positions and lattice structure, many-body collisions
- Currently, electronic stopping determined from SRIM model

- Preliminary calculations of test case: 190 keV He on W
  - Limited statistics: 50k ions
  - Plot A shows backscattered ions (frozen soon after exiting surface at z=0, with target material extending in the positive z-direction)
  - Plot B shows energy distribution of backscattered ions
- Modification of MDRANGE code in progress
  - More efficient output of backscattered ions (computations are fast, but existing output options not designed for backscattering)
  - Aim: obtain full trajectories of backscattered ions
  - Target completion: Oct 2022
- Future work:
  - Include TDDFT-calculated electronic stopping (obtained in D7.1 and D7.2)
  - Experimental ion energies and targets
  - Statistics: >1M ions for each case







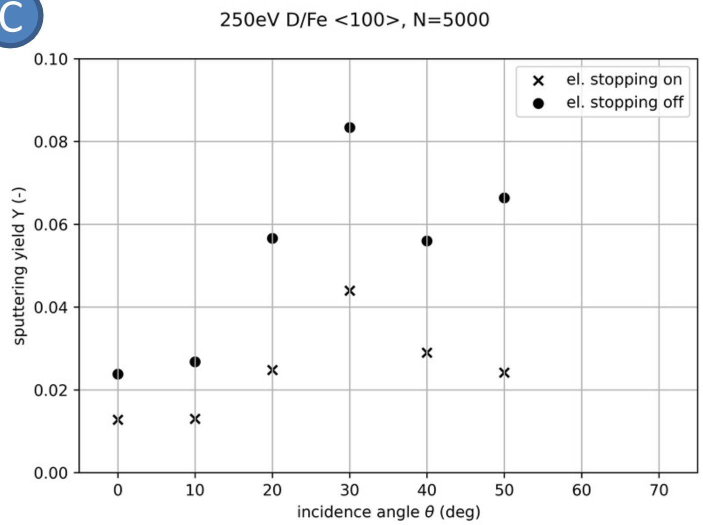
Spatial distribution of backscattered ions

W-P 7: Computational modelling

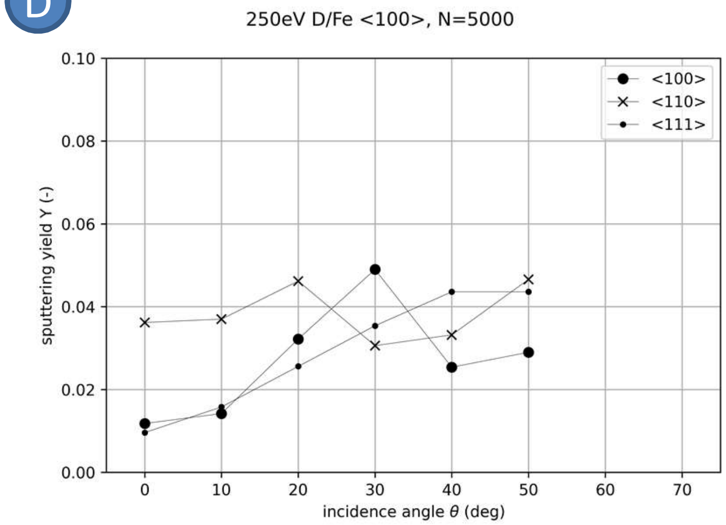
Sputtering with MD simulations (D7.4)

- Classic MD with el. stop. as friction force from SRIM 2013, shown to affect sputtering (plot C)
- Simulation cell: ~16k Fe + 1 D atoms, equilibrated at 300K
- LAMMPS MD code + EAM interatomic potential
- N=5000 Monte Carlo-style simulations per angular step, varying ion azimuthal angle and impact point
- Preliminary results (250eV D on Fe):
  - Plot D: dependence of sputtering yield on ion incidence angle, for 3 low-index orientations (<100>, <110>, <111>) in pristine crystal
- Ongoing work:
  - Additional low-index orientations in pristine crystal (<211>)
  - Uneven surface (step defect, irradiated)

C



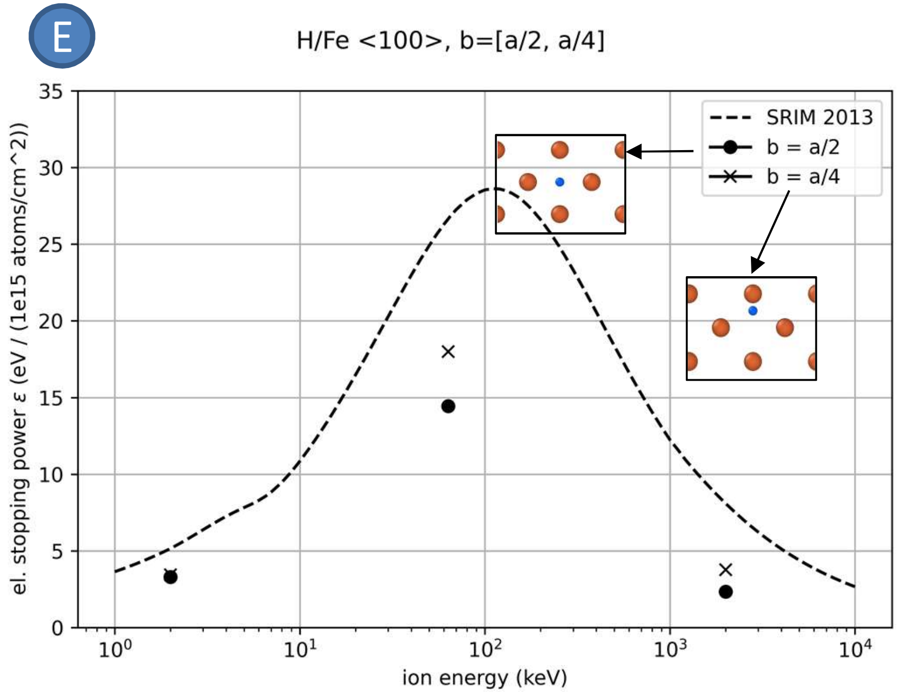
D



W-P 7: Computational modelling

TDDFT electronic stopping power (D7.1)

- Electronic stopping power from rate of change of total energy of the system, with ion travelling at constant velocity
- Simulation cell: 3x3x4 supercell (72 Fe + 1 H atoms), lattice constant ***a***
- Qb@ll TDDFT code + LDA norm-conserving pseudopotentials
- Preliminary results (H on Fe):
    - Plot E: stopping power along <100> channel, for two impact parameters ***b*** and three ion energies
- Ongoing work:
    - Incommensurate trajectories
    - Channeling trajectories with smaller *b*



Summary

Milestones achieved:

2021:

M2.1 → Sample characterization: pristine samples.
M3.1 → Experimental energy loss results from pristine PFCs samples (keV regime).
M5.1 → QCM set-up assembling at UU.

2022:

M2.2 → Sample characterization: damaged samples.
M2.3 → Periodically quality control cross-checks.
M3.2 → Experimental energy loss results from pristine PFCs samples (sub-keV regime).

Summary

In progress:

2022:
M5.1 → Comparisons on the experimental sputtered yields between pristine Fe, W, EUROFER samples to Monte Carlo-based BCA simulations using input data from energy loss and interatomic potential.

M7.1 → Ab-initio calculations for energy loss and comparison to results: pristine samples.
M7.3 → Implementation of geometrically dependent electronic energy losses in the MDRANGE ion range code.

Summary

Future milestones (2023 & 2024):

M3.3 → Experimental data from damaged W & Fe.
M3.4 → Experimental data from damaged EUROFER.

M4.1 → Determination of short-range interactions from experimental spectra and BCA calculations.
M4.2 → Comparison of the short range interactions for pristine vs. damaged samples: defects influence.

M5.2 → Benchmarking sputtering yield codes with input data from WP3 and WP4.
M5.3 → Evaluate how sensitive the sputtering yield is in terms of energy loss and interatomic potential when local defects and impurities (i.e. damaged samples) are present.

M6.2 → Depth profile of the irradiated Fe, W and EUROFER samples suitable for WP4.

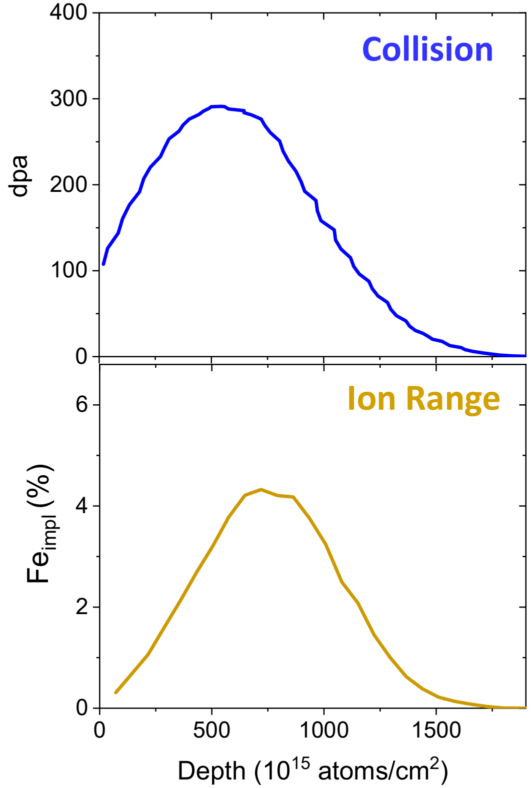
M7.2→ Ab-initio calculations of damaged samples and comparison to experiments: local effects on the fundamental quantities.
M7.4 → Comparisons of predicted and experimentally measured electron energy losses for input into MD based simulations.
M7.5 → Experimentally deduced short range interactions as inputs for MD based simulations of sputtering yield.

Extras

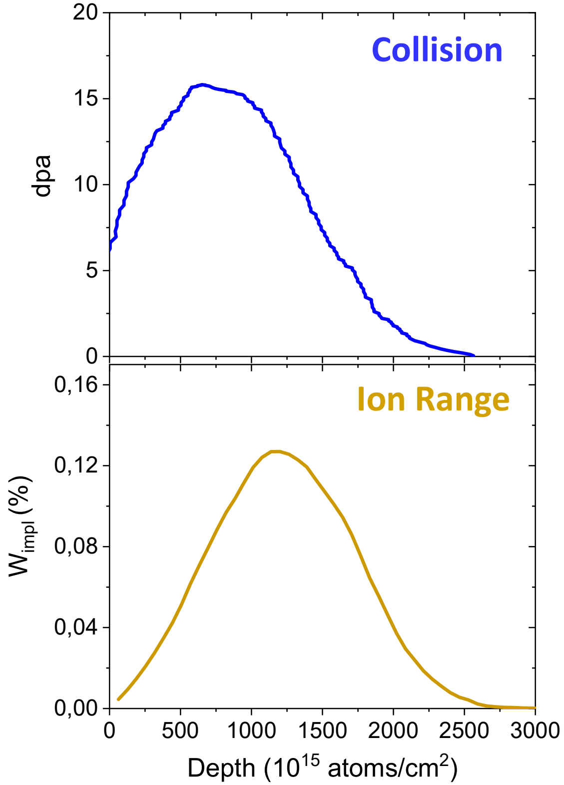
W-P 6: Ion-irradiation experiments

TRIM simulations

Fe^+ 300 keV → Fe, EUROFER, Si samples
Fe areal density: 42.25×10^{15} Fe/cm^2

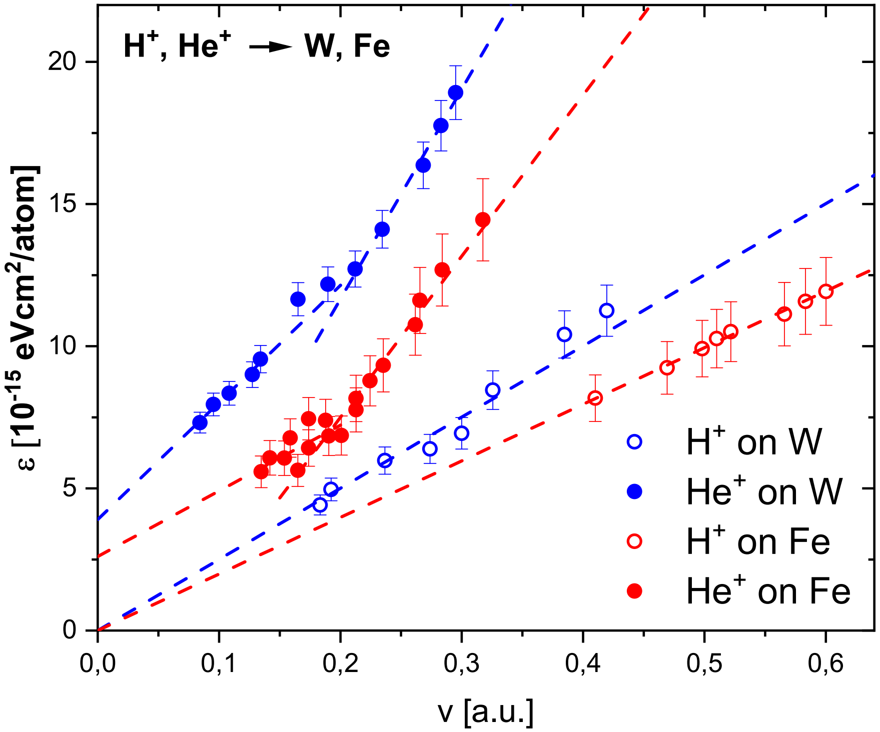


W^{2+} 2.84 MeV → W and Si samples
W areal density: 1.57×10^{15} W/cm^2



W-P 3: Electronic energy loss measurements

H and He on Pristine Fe and W: Velocity dependence in low energy range



FEG → $S_e = Q(Z_1, r_s)v$

H → W, Fe

→ SCS scales with velocity.

He → W, Fe

→ Strong deviation of $\varepsilon \propto v$ at ~0.2 a. u.

→ Positive offset on y axis:

→ Similar behaviour observed on He → Pt [1]

→ Attributed to charge-exchange processes between He^{+} and target with non-linear velocity dependence.

[1] D. Goebl, D. Roth, and P. Bauer, Phys. Rev. A, 87, 062903 (2013).