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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Monitoring of 2023 Enabling Research activities, 06th of February 2024

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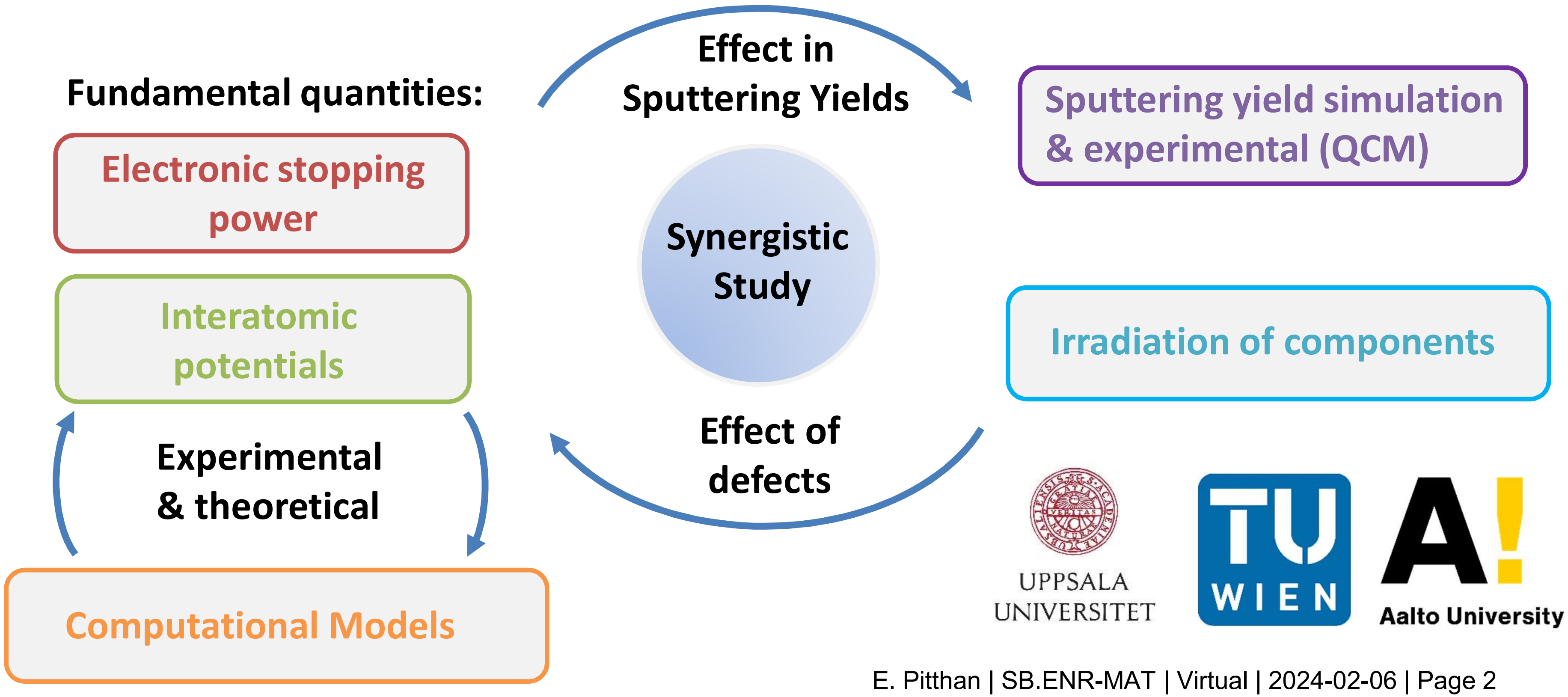
Aim

To investigate underlying **quantities fundamental** for **sputtering** and **defect formation** from plasma-wall interaction: important input variables in modelling of **erosion** and **implantation** in plasma facing components.



UPPSALA UNIVERSITET

TU WIEN

Aalto University

Team 2023

VR	ÖAW	VTT
Eduardo Pitthan (PI)	Martina Fellinger	Andrea Sand
Jila Shams-Latifi	Johannes Brötzner	Evgeniia Ponomareva
Philipp M. Wolf	Christian Cupak	Ludovico Caveglia Curtil
Petter Ström	Richard Wilhelm	Tetiana Malykhina
Per Petersson	Friedrich Aumayr	Akseli Aro

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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Main observations from 2021 & 2022

- Experimental stopping power measurements (**SCS**) for H and He in W, Fe and EUROFER97:

  Pronounced discrepancies between SRIM-2013 and new experimental data in the low energy regime were observed: up to 20% for protons and 26% for He in Fe and up to 20% for protons and 60% for He in W.

  → **Confirm with different approach (absolute with deposited films).**

  → **Compare with SCS from TDDFT (theoretical).**

- Binary Collision Approximation (BCA) simulations highlight **effect of SCS in sputtering yields.**

- Molecular Dynamic (MD) simulations indicate **clear dependence of crystalline orientation in sputtering yields**, while surface irregularities had negligible effect.

  Possible explanation for sputtering yield experimental observations.

Deliverables and milestones proposed for 2023:

W-P 1: General management

D1.4 → Annual meeting (2023)
M1.3 →M1.3: Annual Report (due date: 2023-12-31)

W-P 2: Sample preparation

M2.3 → Periodically quality control cross checks (Done by ToF-ERDA → No increase of contamination).

W-P 3: Electronic energy loss measurements

D3.3 → Stopping power of damaged PFCs samples for light ions (MEIS regime).
M3.3 →Experimental data from damaged W & Fe.
D3.4 (to complete in 2024) → Stopping power of damaged PFCs samples for light ions (LEIS regime).

W-P 4: Interatomic potential measurements

M4.1 → Determination of short range interactions from experimental spectra and BCA calculations.
D4.3 (to complete in 2024) →ToF-LEIS/MEIS angular scans measurements (damaged).

Deliverables and milestones proposed for 2023:

W-P 5: Sputtering yield & QCM

D5.3 → Sputtering yields and angular distributions of damaged W and EUROFER97 samples.

M5.2 →Benchmarking sputtering yield codes with input data from W-P 3 and W P 4.

W-P 6: Ion-irradiation experiments

D6.2 → Ex-situ ion irradiation experiments on the PFCs samples at UU.

D6.3 → In-situ ion-irradiation experiments on the PFCs samples TU.

D6.4 (to complete in 2024) → In-situ ion irradiation experiments on the PFCs samples UU.

M6.2 (to complete in 2024) →Depth-profile of the irradiated Fe, W and EUROFER samples suitable for W P4.

W-P 7: Computational modelling

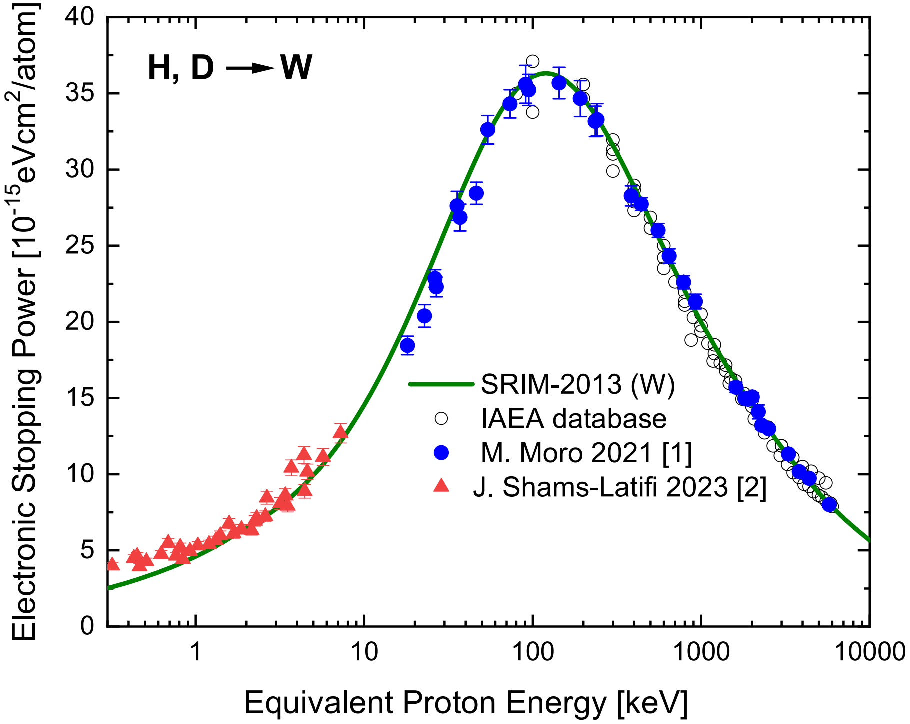
D7.3 (started earlier) →MDRANGE simulations of ion implantation ranges and sputtering yields from surfaces with evolving composition.

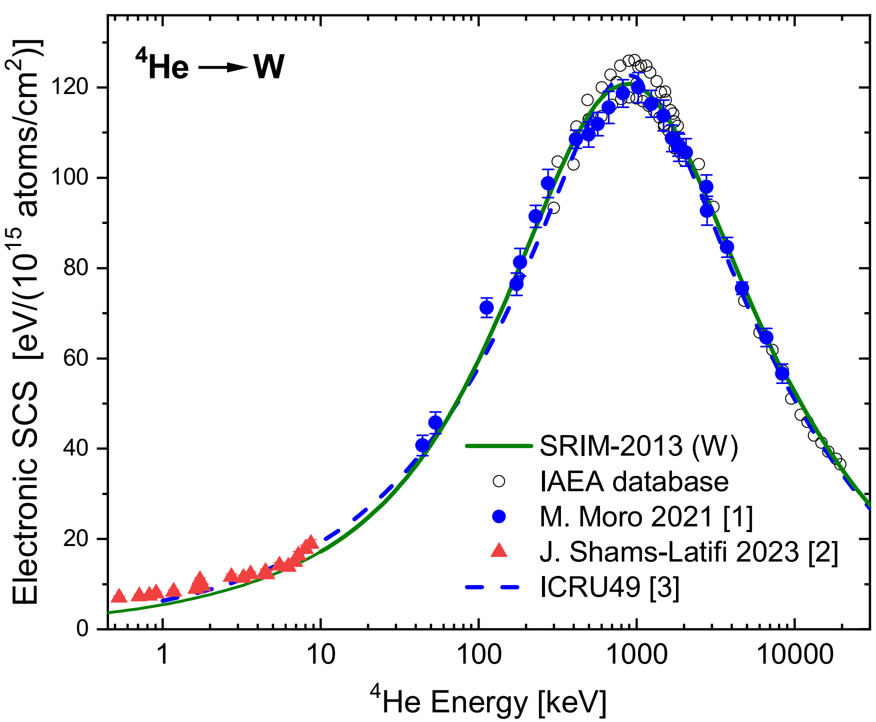
D7.4 (started earlier) → D7.4: MD simulations, including electronic energy losses within a two temperature formalism of sputtering from complex surfaces.

W-P 3: Electronic energy loss measurements

Data and analysis: J. Shams-Latifi. P. M. Wolf, and E. Pitthan

Experimental stopping cross-section of pristine and sputter-deposited W (relative and absolute approach):





[1] M. V. Moro et al., Nucl. Instrum. Meth B **498** (2021).
[2] J. Shams-Latifi, et al., Nucl. Mater. and Energy **36** (2023).
[3] M. J. Berger, et al., Report 49, Oxford Academic (1993).

W-P 3: Electronic energy loss measurements

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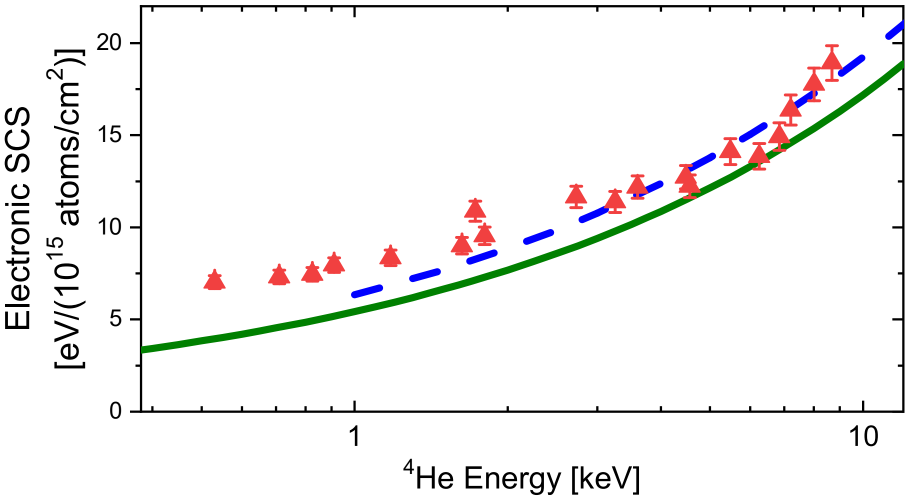
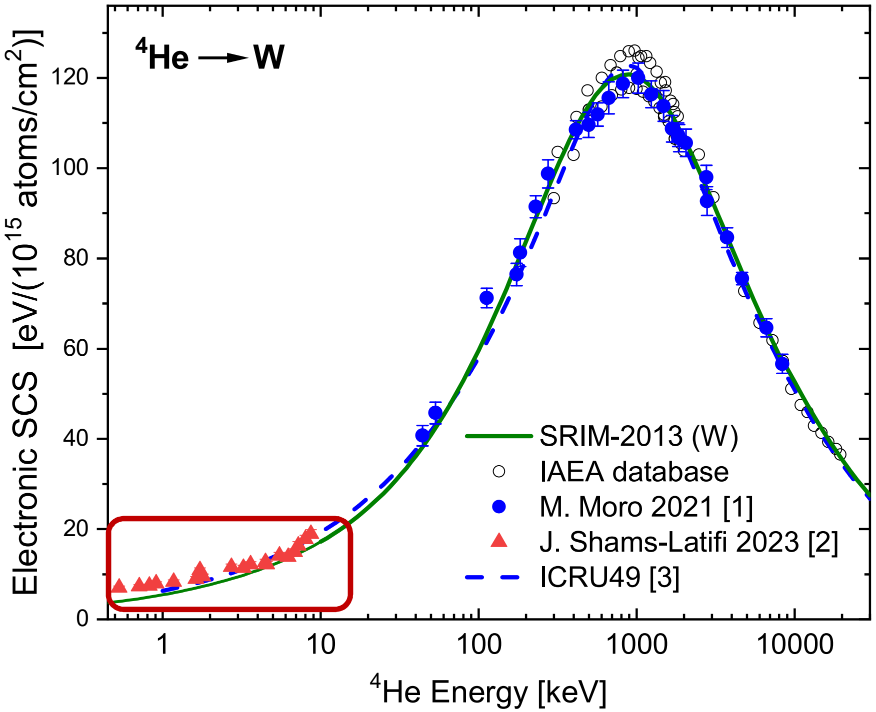


SCS at LEIS published [2]:
LEIS: Discrepancies from SRIM-2013 up to 20% for protons and 60% for He.



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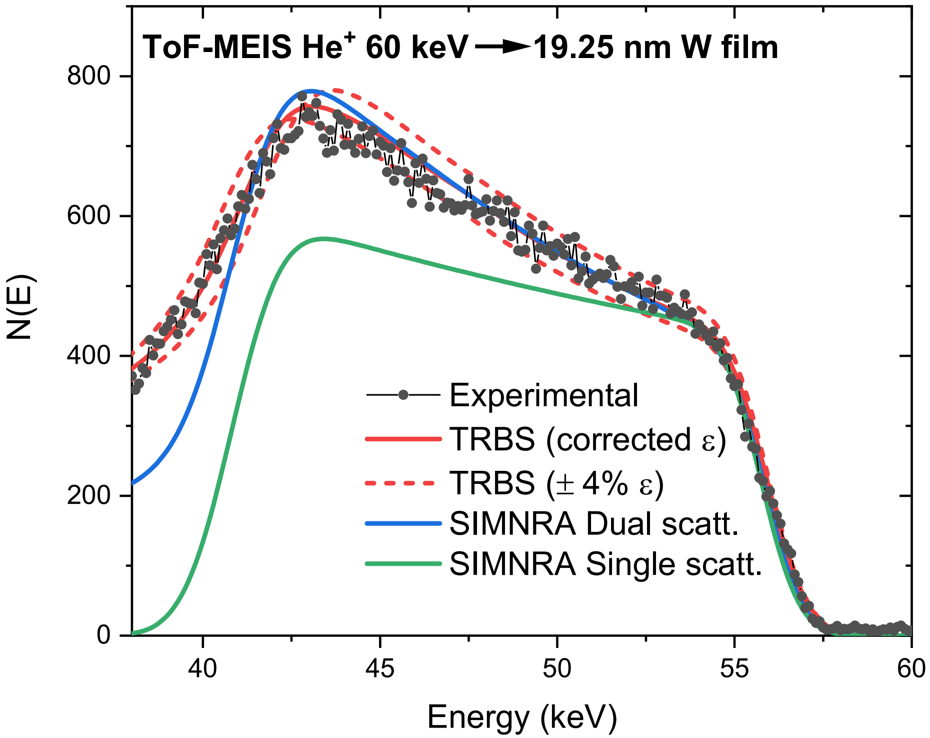
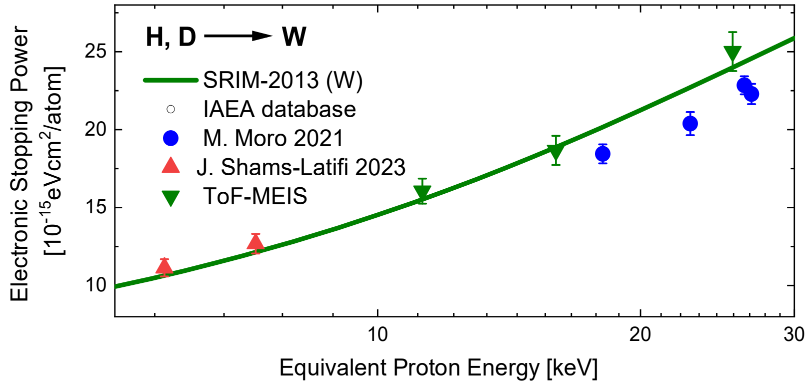
[2] J. Shams-Latifi, et al., Nucl. Mater. and Energy **36** (2023).
[3] M. J. Berger, et al., Report 49, Oxford Academic (1993).

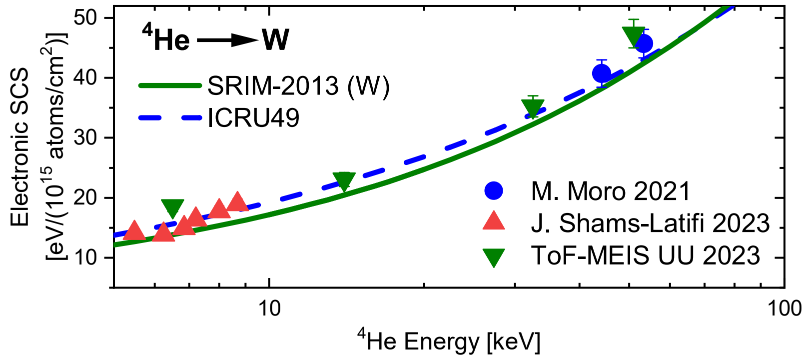
W-P 3: Electronic energy loss measurements

Data: R. Holenak, J. Shams-Latifi, E. Pitthan. Analysis: E. Pitthan

Experimental stopping cross-section of sputter-deposited W (ToF-MEIS 5-60 keV for H_2^+ and He^+)







SCS at MEIS: Good agreement with SRIM for protons and with ICRU for He.

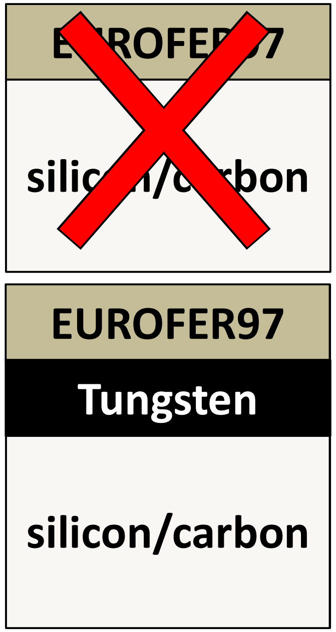
W-P 3: Electronic energy loss measurements

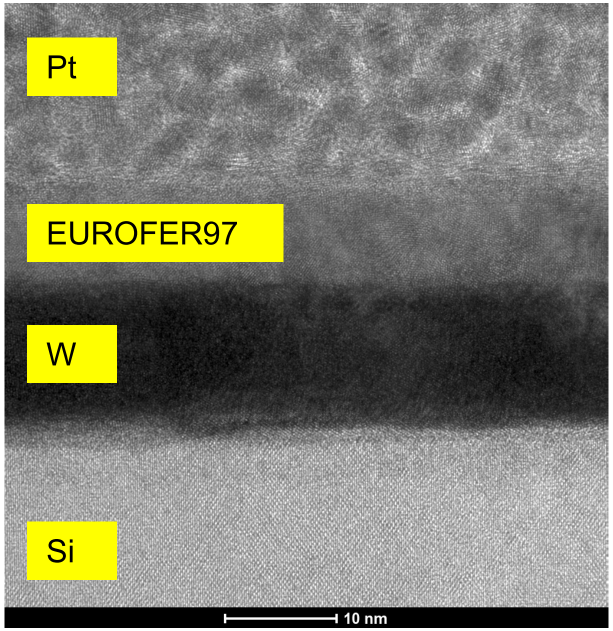
Data and Analysis: J. Shams-Latifi

Experimental stopping cross-section of sputter-deposited EUROFER97 for LEIS (In-progress)

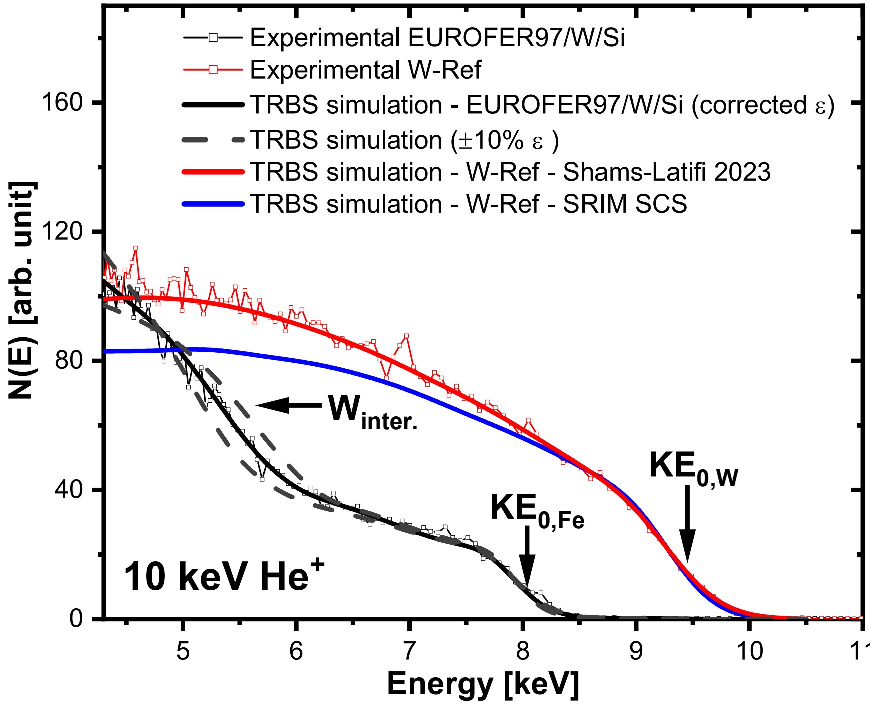
→ Analysis from spectrum height or spectrum width unfavorable for compound systems and lighter species.

→ Surface interface segregation is a risk – best to look on the signal indirectly – via a marker layer.





Characterization of re-deposited PFM structures (pinboard 36144):
J. Shams-Latifi, E. Pitthan, et. al Mater. Res Express. 11 (2024) 016518.



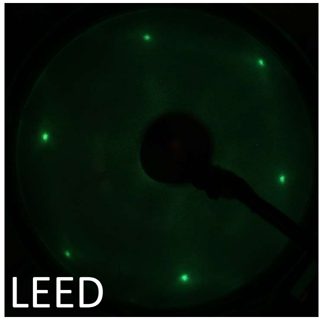
W-P 4: Interatomic potential measurements

Data and analysis: P. M. Wolf

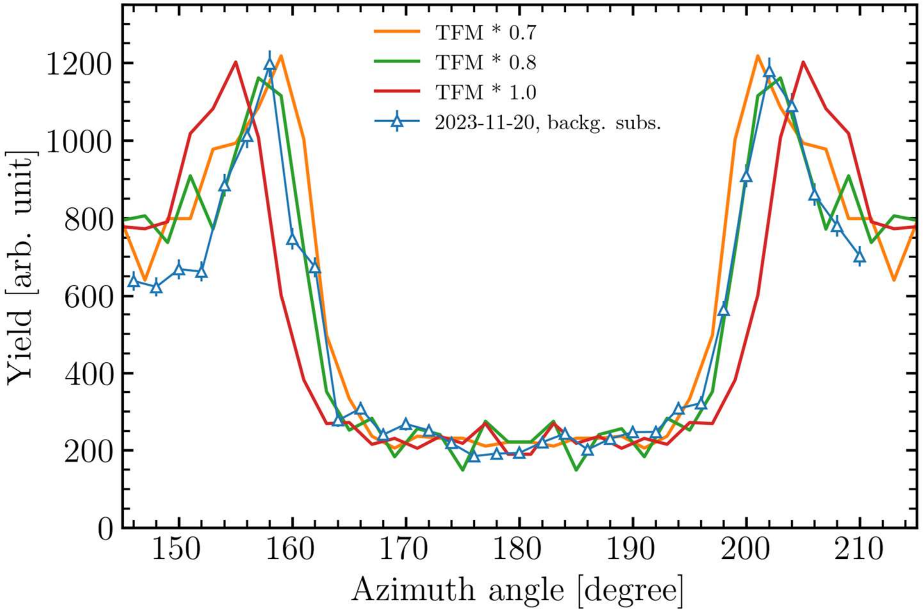
3 keV He – angular scans on W(110)

Aim: Determining the screening length correction factor.

The surface shows no reconstruction according to LEED.



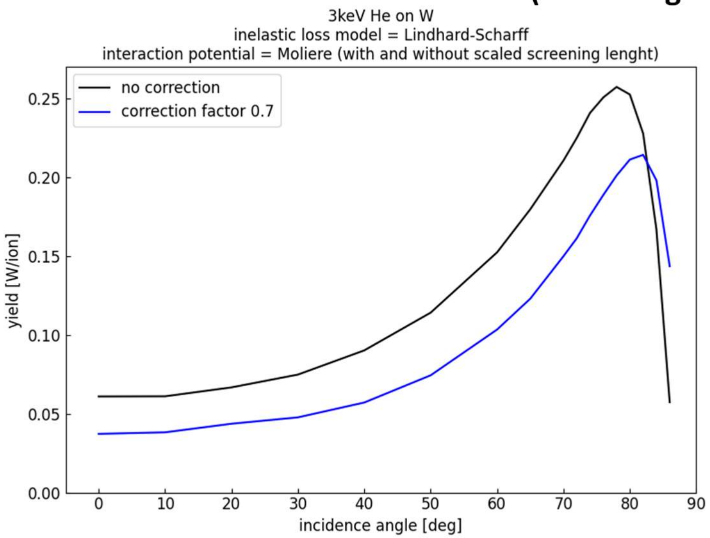
He in W(110) → c_a= 0.8 [TFM]
D in W(110) → c_a= 1.0 [TFM]



- **Thomas-Fermi-Moliere potential:**

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

- With screening length $a = ca \cdot af$, a_f is the Firsov screening length and c_a a correction factor.
- In the Kalypso (molecular dynamics) simulation the interatomic potential is changed using the correction factor.
- **Effect on SY simulations in SDTrimSP (M. Fellinger):**



W-P 5: Sputtering yields and BCA simulation

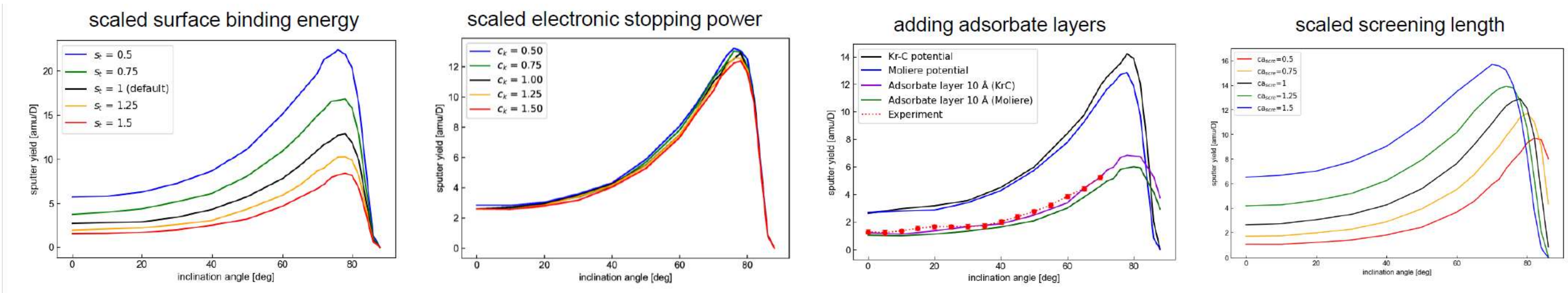
Data and analysis: M. Fellinger

Systematic investigation of effect of nuclear data corrections in sputtering yield simulations.

SDTrimSP example case: 1 keV D on Eurofer, Lindhard-Scharff stopping model, Moliere interaction potential.

Scaling electronic stopping power;
Surface binding energy;
Adsorbate layer thickness;
→global offset in sputtering yields

Screening length in interatomic potential.
→offset in sputtering yieds
→ Shifted maximum in yields over angle curve



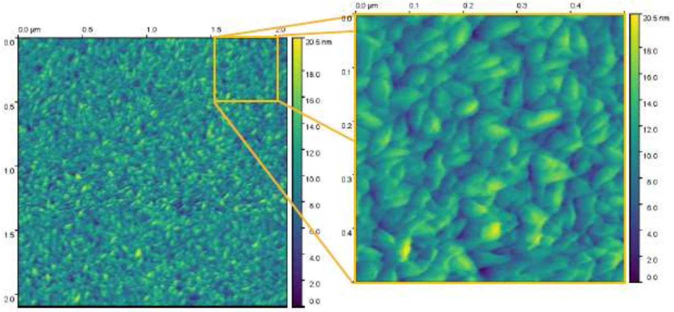
W-P 5: Sputtering yields and BCA simulation

Sample preparation: E. Pitthan; Data and analysis: M. Fellinger

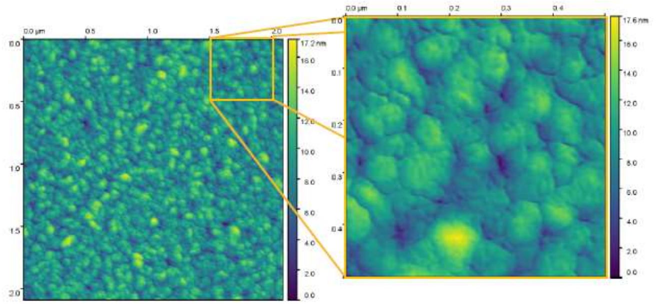
Sputtering Properties of self-irradiated EUROFER97:

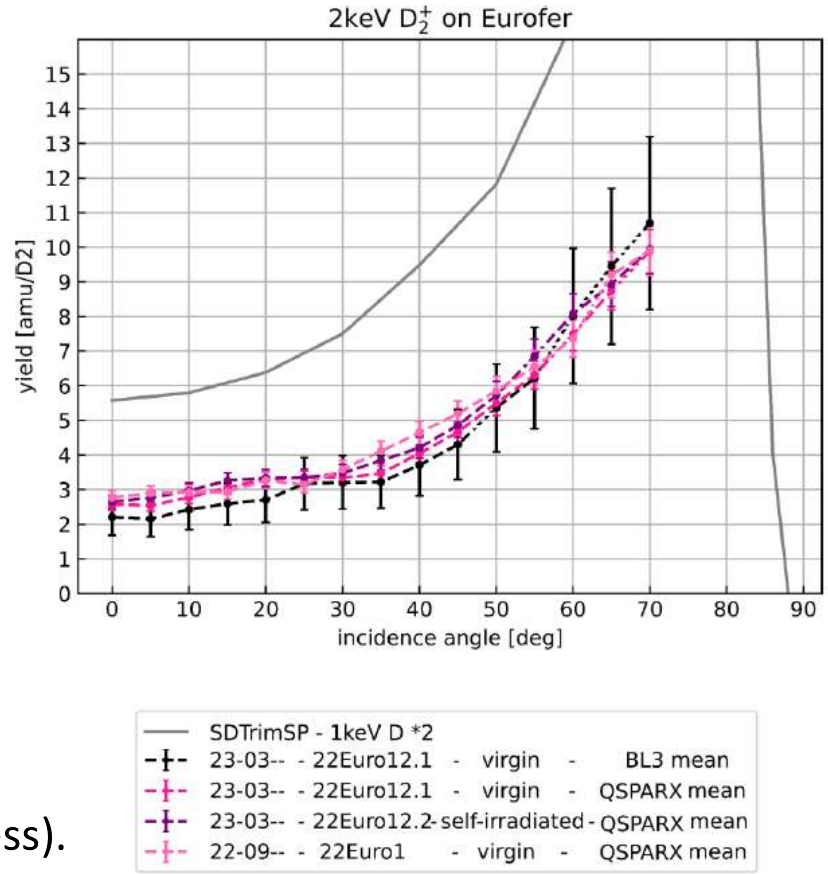
Fe^+ 300 keV (37×10^{15} Fe/cm^2) → deposited EUROFER97/QCM

AFM before Fe^+ irradiation:



AFM after Fe^+ irradiation:





No significant effect of self-irradiation in SY (in progress).
Similar approach for W.

W-P 6: Ion-irradiation experiments

Data and analysis: T. T. Tran, E. Pitthan

Experimental (preparation for WP-3 and 5)

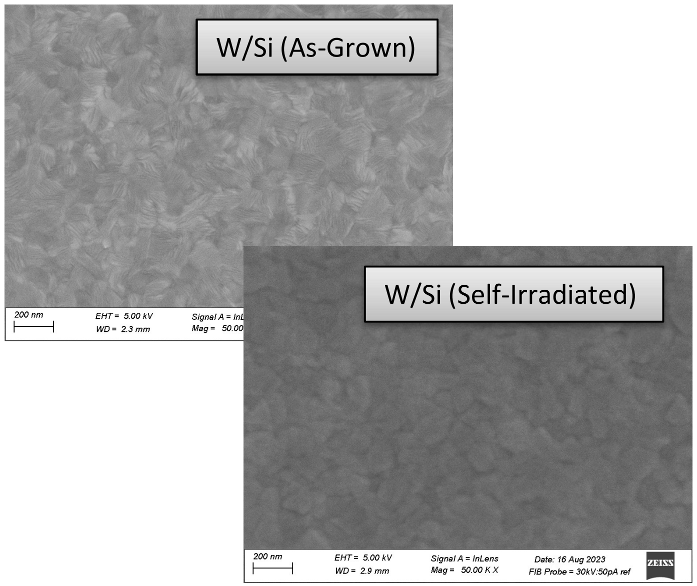
Sample: W(300 nm)/(Si, C, QCM)

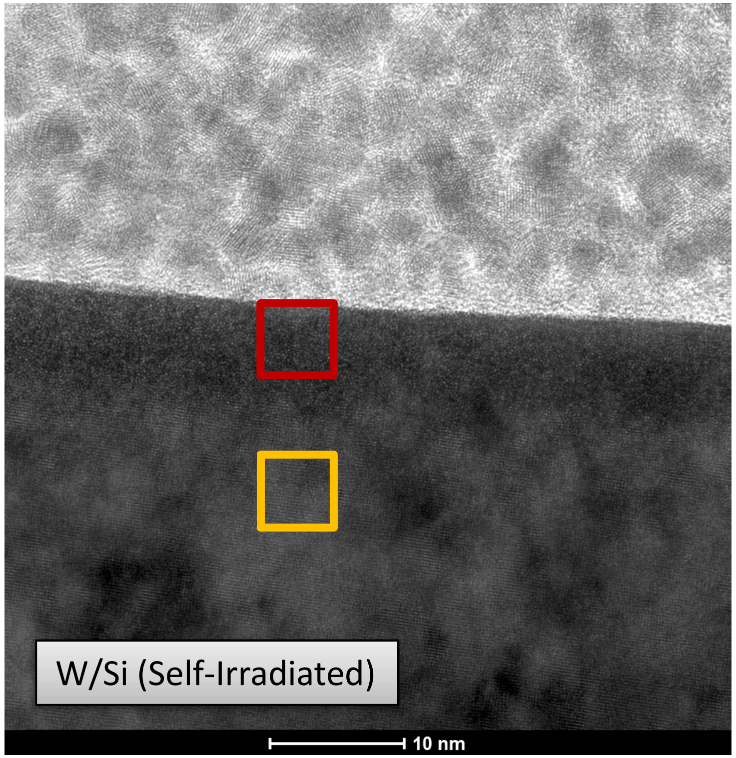
Implantation: W^{2+} 600 keV

Fluence: 1.5×10^{15} atoms/cm^2

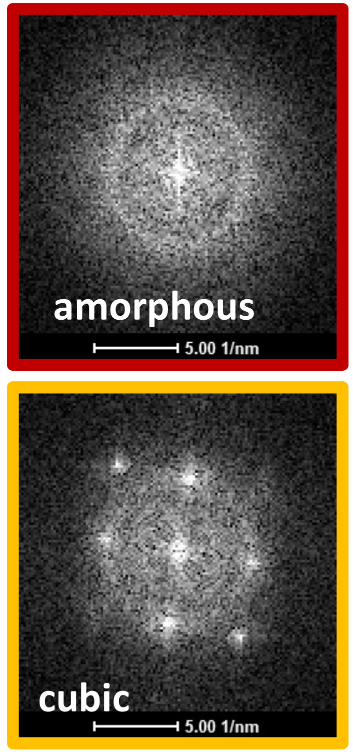
SEM: *Smoothening of surface after Implantation.*

TEM: *amorphization of surface.*





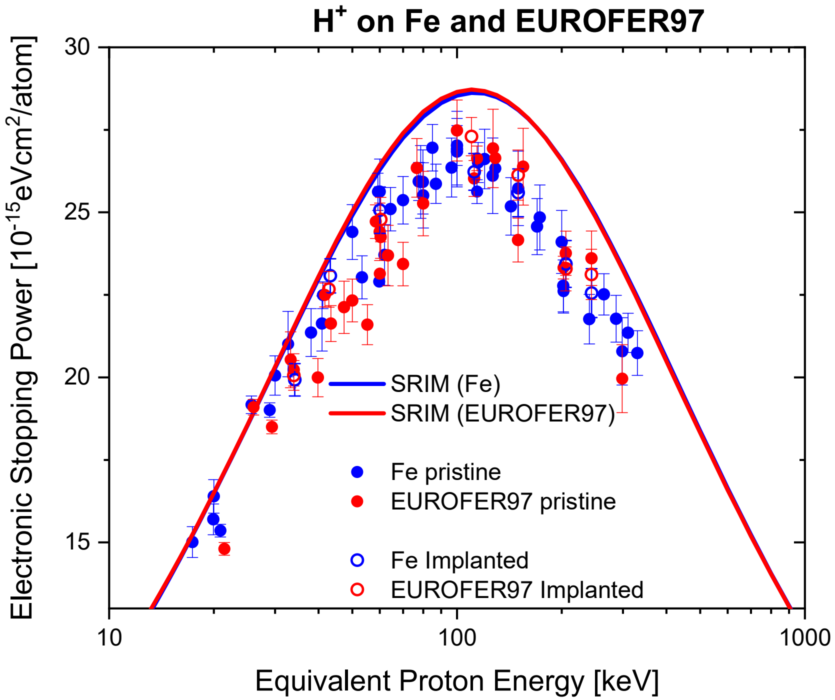
FFT:

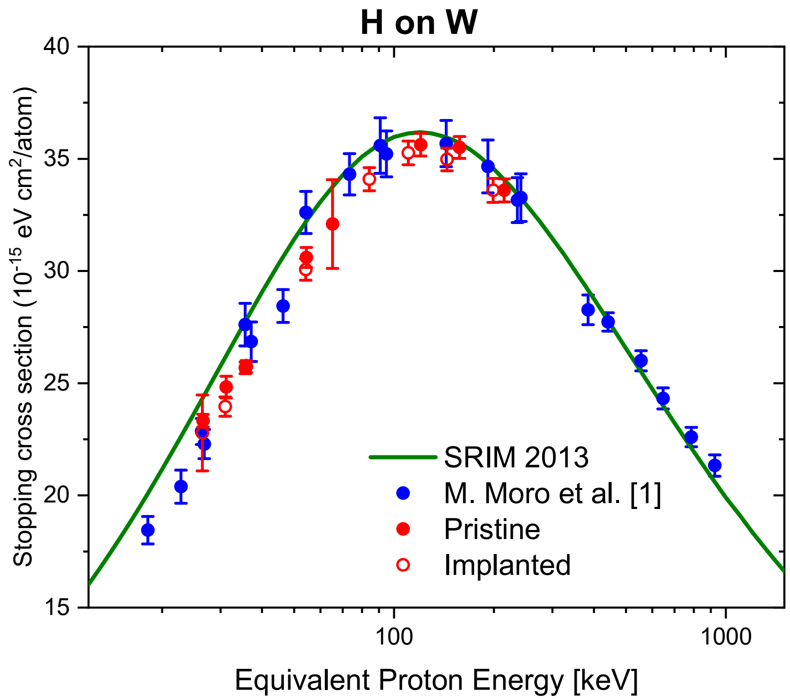


W-P 6: Ion-irradiation experiments

Data and analysis: E. Pitthan

Ion damaged by self-irradiation →*Fe, EUROFER97, W SCS irradiated samples*





→ No significant difference/trend on SCS from Pristine and Irradiated samples.

→ Measurements at lower energies are in progress.

W-P 7: Computational modelling

Data and analysis: E. Ponomareva, A. Sand

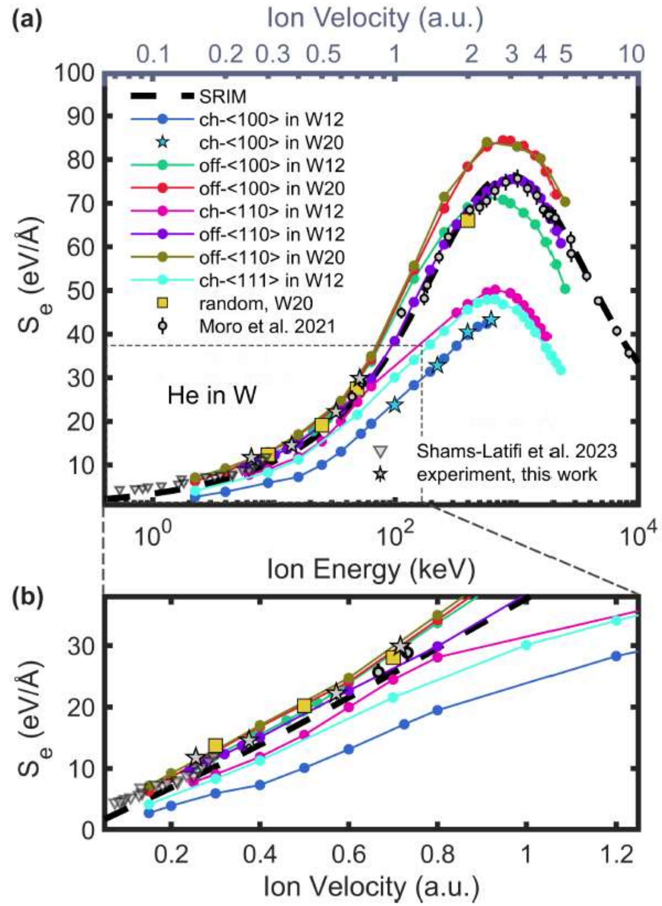
D7.1: Ongoing. Theoretical calculation of electronic stopping power for random trajectories of light ions in pristine W, Fe and Fe-alloys using TD-DFT calculations.

Systematic investigation of the influence of **ion-target geometry** (channelling, off-centre, and random geometries) and **core-states description** (W12 and W 20) of the target in the electronic energy losses.

Method for selecting **random trajectories** to optimize convergence efficiency completed. Good agreement with experimental data at lower energies.

Joint manuscript (Aalto and UU) submitted to publication (pinboard 36768).

Final steps for Fe and Fe-alloys (additional calculations for low energies).



W-P 7: Computational modelling

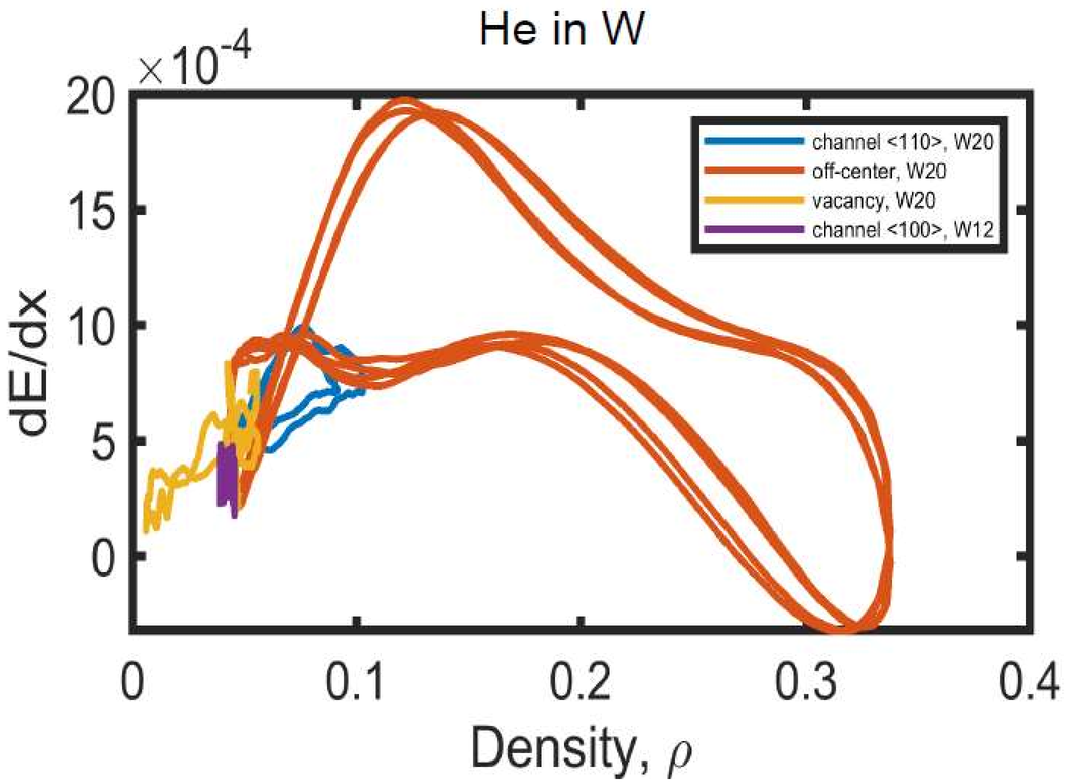
Data and analysis: E. Ponomareva, A. Sand

TDDFT calculations of electronic stopping power for different trajectories of light ions in the presence of defects (vacancies).

Provides data on dissipation in different local environments, for use in fitting the electron density-dependent coupling function.

Approach:
Two-temperature MD framework
Electronic density dependent (ρ).

No significant effect of vacancies in electronic stopping power in agreement with experimental data.



W-P 7: Computational modelling

Data and analysis: L. Caveglia Curtil, A. Sand

Sputtering with MD simulations (D7.4)

- Workflow optimized and benchmark simulations with SRIM stopping powers completed.
- Effect of surface orientation (paper under preparation with TUWien).
- Effect of surface roughness (step defect).
- Fitting of ion-electron coupling for two temperature model simulations with environmentally dependent stopping power in progress.

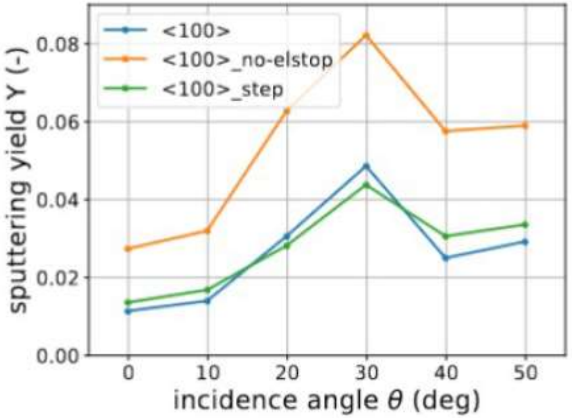
Main observations:

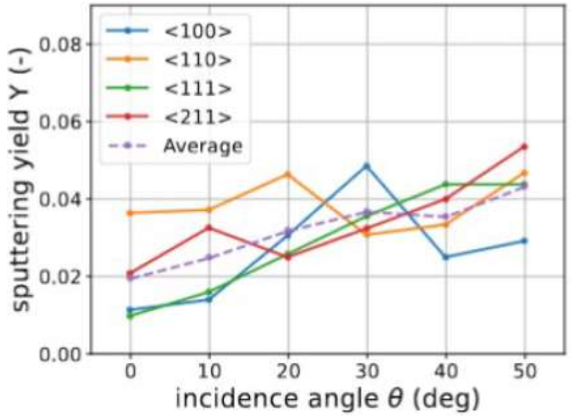
→Dependence on surface orientation.

→ Negligible effect of unevenness of surface

→ (step-defect).

250 eV D on Fe





Summary of main results from 2023

New SCS results confirm the discrepancies between commonly used semi-empirical models (SRIM) up to 60% for the case of helium in tungsten. Experimental data was published this year (pinboard 35412).

Simulations using Time-Dependent Density Functional Theory (TD-DFT) present good agreement with experimental data at low-energy regimes and describes the strong influence of ion-target geometry and core-states description of the target in the electronic energy losses. A manuscript was submitted (pinboard 36768).

Main effect of irradiation on samples was the amorphization of surface region, while no significant modification on energy losses and sputtering yields was observed in comparison to pristine samples. TD-DFT calculations of electronic energy losses in the presence of defects (vacancies) support the experimental observations.

Experimentally deduced correction factor for interatomic potential of light ions in W at low energies were obtained. Sputtering yield simulations using binary collision approximation (SDTrimSP) indicates that interatomic potential corrections have a strong impact in the sputtering yield simulations.

Molecular dynamic calculations of sputtering yields were completed for deuterium and helium in Fe and W and compared to the ones obtained experimentally in this project. Results describes in detail the strong influence of surface orientation in sputtering yields. A manuscript is currently in preparation.

Main activities proposed for 2024

Continue the experimental investigation of the stopping power of damaged PFCs samples for light ions with focus in the LEIS energy regime.

Continue with ToF-LEIS angular scans measurements for Fe(100).

Continue simulations of sputtering yield and angular distributions of sputtered atoms of damaged (self-irradiated) PFCs.

Continue electronic energy losses within a two temperature formalism of sputtering.

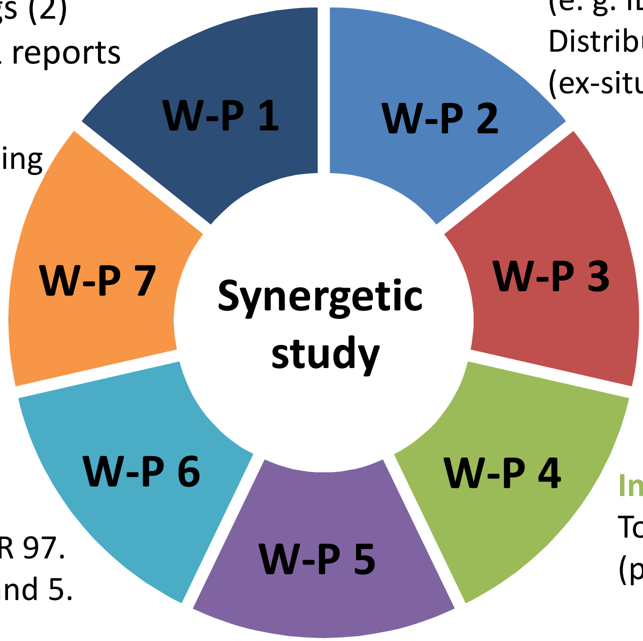
Extras

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.

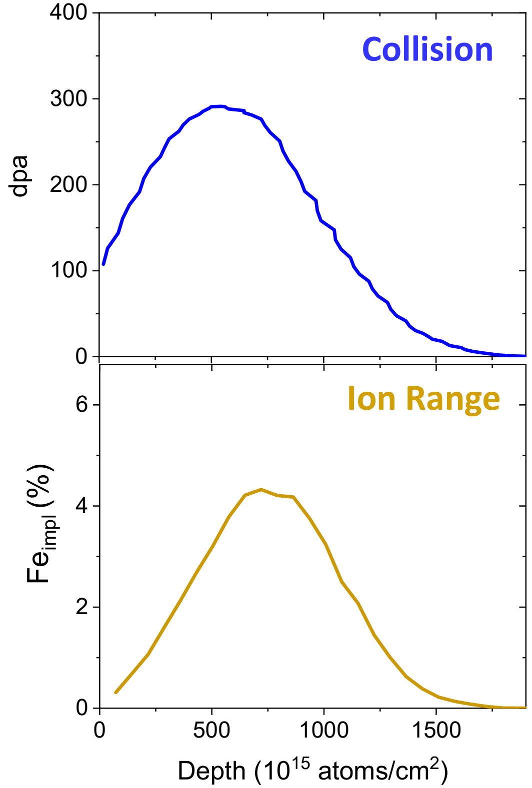
Interatomic potential measurements
ToF-LEIS & ToF-MEIS angular scans measurements (pristine and damaged samples).

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).

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