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TECHNISCHE UNIVERSITÄT WIEN

Aalto University School of Science

EUROfusion Horizon Europe
(2021-2023)

ENABLING RESEARCH PROJECT

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

Monitoring of 2021 activities
1st of December 2021

https://wiki.euro-fusion.org/wiki/Project_No5

https://indico.euro-fusion.org/category/305/

Outline

- Aim;
- Working-packages & schedule;
- Main results obtained & work in progress;
- Achievement of Scientific Deliverables foreseen for 2021;
- Activities foreseen for 2022.

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

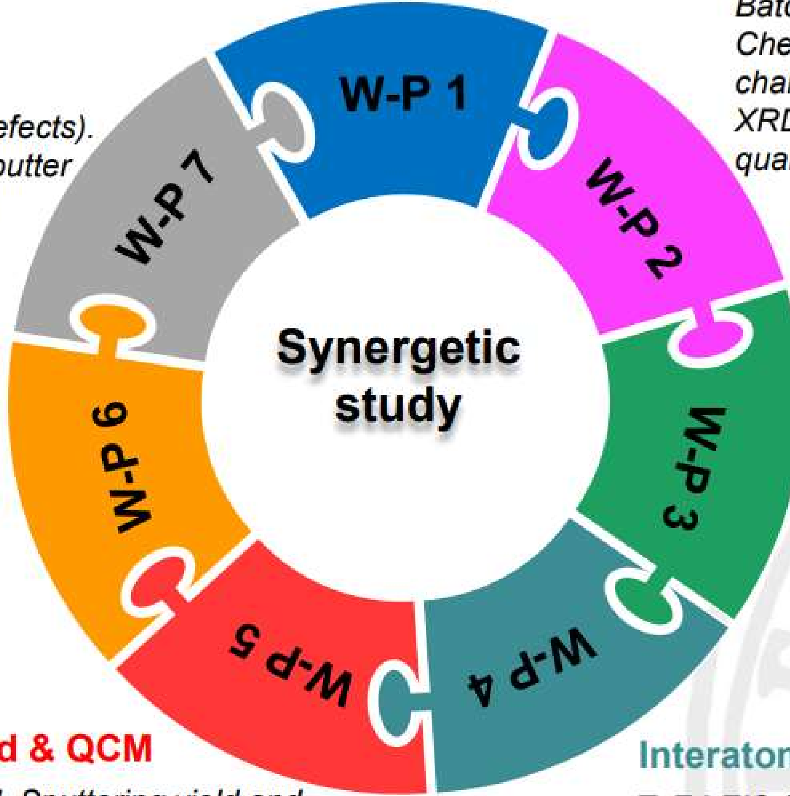
Kick-off meeting
Task coordination
Annual meetings (2)
Final meeting & reports

Sample preparation

Batches of Fe, W and EUROFER. Chemical and morphological characterization (e.g., AFM, SEM, XRD). Distribution and routinely quality control (ex-situ and in-situ).

Computational modeling

TDDFT simulations of electronic stopping power of W, Fe and EUROFER-like (samples w/wo defects). MDRANGE: ion implantation & sputter yield (input: electronic stopping)



Electronic energy loss meas.

Experimental stopping cross section of pristine Fe, W and EUROFER. For each sample @ keV and sub-keV regime. Compare experimental results between pristine & damaged

Ion-irradiation experiments

Define irradiation conditions. Ex-situ and in-situ ion irradiation experiments on Fe, W and EUROFER @ UU and TU. Samples to be reused in W-Ps 3,4,5

Sputtering yield & QCM

QCM set-up at UU. Sputtering yield and angular distributions of pristine Fe, W and EUROFER samples (@ TU and @ UU up to some extend). BCA-based simulations (SDTrimSP).

Interatomic potential measurements

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

Schedule

Updates: Deliverables and Milestones per calendar year

Table: Revised deliverables (D) and milestones (M) schedule according to the working-packages (W-Ps) per calendar year.

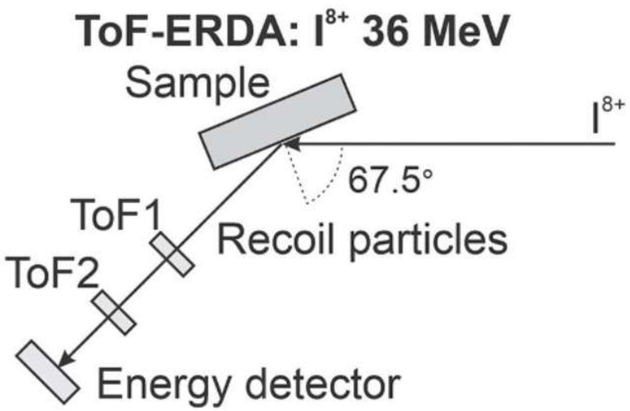
<table>
<tr><th></th><th colspan="2">2021</th><th colspan="4">2022</th><th colspan="4">2023</th><th colspan="2">2024</th></tr>
<tr><th>W-Ps</th><th>5-8</th><th>9-12</th><th>1-3</th><th>4-6</th><th>7-9</th><th>10-12</th><th>1-3</th><th>4-6</th><th>7-9</th><th>10-12</th><th>1-2</th><th>3-4</th></tr>
<tr><td>W-P 1: General management</td><td>D1.1</td><td>D1.2
M1.1</td><td></td><td></td><td></td><td>D1.3
M1.2</td><td></td><td></td><td></td><td>D1.4
M1.3</td><td></td><td>D1.5
M1.4</td></tr>
<tr><td>W-P 2: Sample preparation/ characterization</td><td colspan="4">D2.1, D2.2, D2.3, D2.4, D2.5
M2.1</td><td></td><td>M2.2
M2.3</td><td></td><td>M2.3</td><td></td><td></td><td>M2.3</td><td></td></tr>
<tr><td>W-P 3: Electronic energy loss measurements</td><td colspan="2">D3.1</td><td>M3.1</td><td colspan="2">D3.2</td><td>M3.2</td><td colspan="2">D3.3</td><td>M3.3</td><td colspan="2">D3.4</td><td>M3.4</td></tr>
<tr><td>W-P 4: Interatomic potential measurements</td><td></td><td></td><td>D4.1</td><td colspan="3">D4.2</td><td>M4.1</td><td colspan="4">D4.3</td><td>M4.2</td></tr>
<tr><td>W-P 5: Sputtering yields and BCA simulations</td><td colspan="3">D5.1</td><td>M5.1</td><td colspan="2">D5.2</td><td colspan="2">D5.3</td><td>M5.2</td><td colspan="3">D5.4
M5.3</td></tr>
<tr><td>W-P 6: Ion irradiation experiments</td><td></td><td colspan="3">D6.1</td><td>M6.1</td><td colspan="2">D6.2</td><td colspan="2">D6.3</td><td colspan="2">D6.4
M6.2</td><td></td></tr>
<tr><td>W-P 7: TD-DFT and Molecular dynamics</td><td></td><td colspan="2">D7.1</td><td>M7.1</td><td colspan="2">D7.2</td><td>M7.2</td><td>D7.3
M7.3</td><td>D7.4
M7.4</td><td>D7.4</td><td colspan="2">D7.4
M7.5</td></tr>
</table>

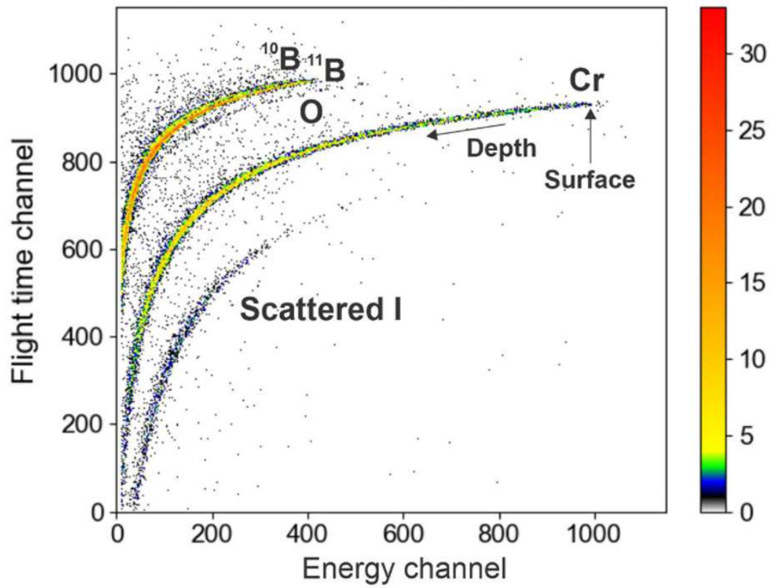
Working-packages

Sample preparation

- **Working-package 2 (W-P 2) main deliverables/milestones for 2021:**

→ 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.





E. Pitthan, M. V. Moro, S. A. Correa, D. Primetzhofer, *Surf. Coat. Tech.* **417,** 127188 (2021)

Electronic Stopping Power

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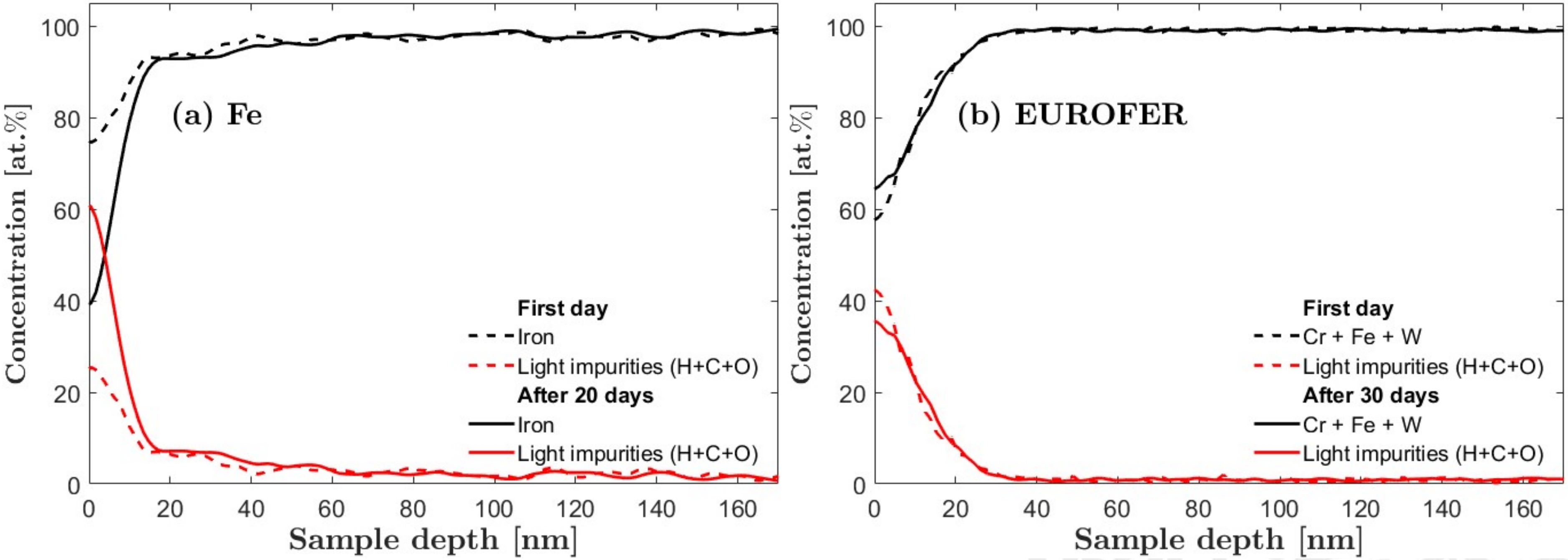
Stopping data for Fe & EUROFER in the medium/low energy regime

Sample characterization



Final stopping data corrected by Bragg's rule

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

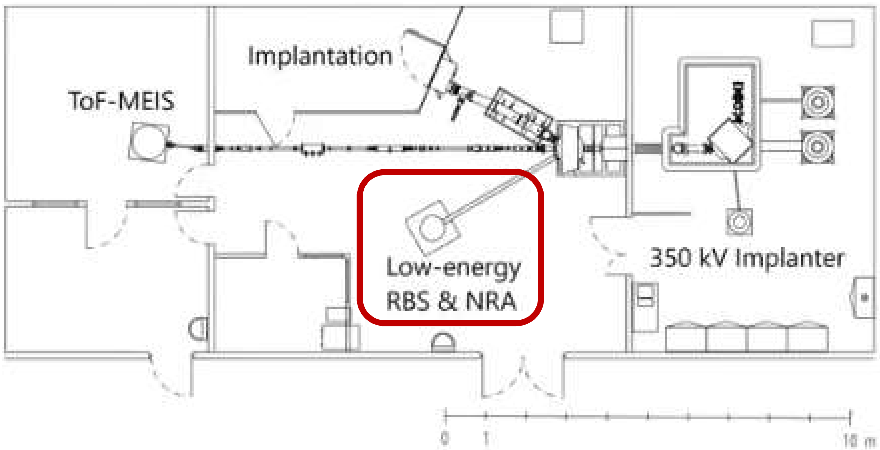
Working-packages

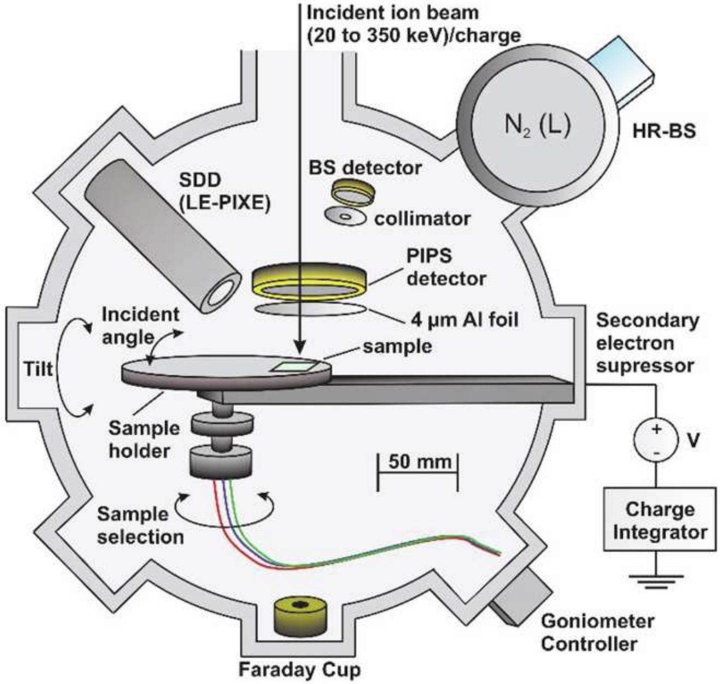
Electronic energy loss measurements

- **Working-package 3 (W-P 3) main deliverables/milestones for 2021:**

→ Stopping power of pristine PFCs samples for light ions (keV regime).

350 kV Danfysik Implanter:

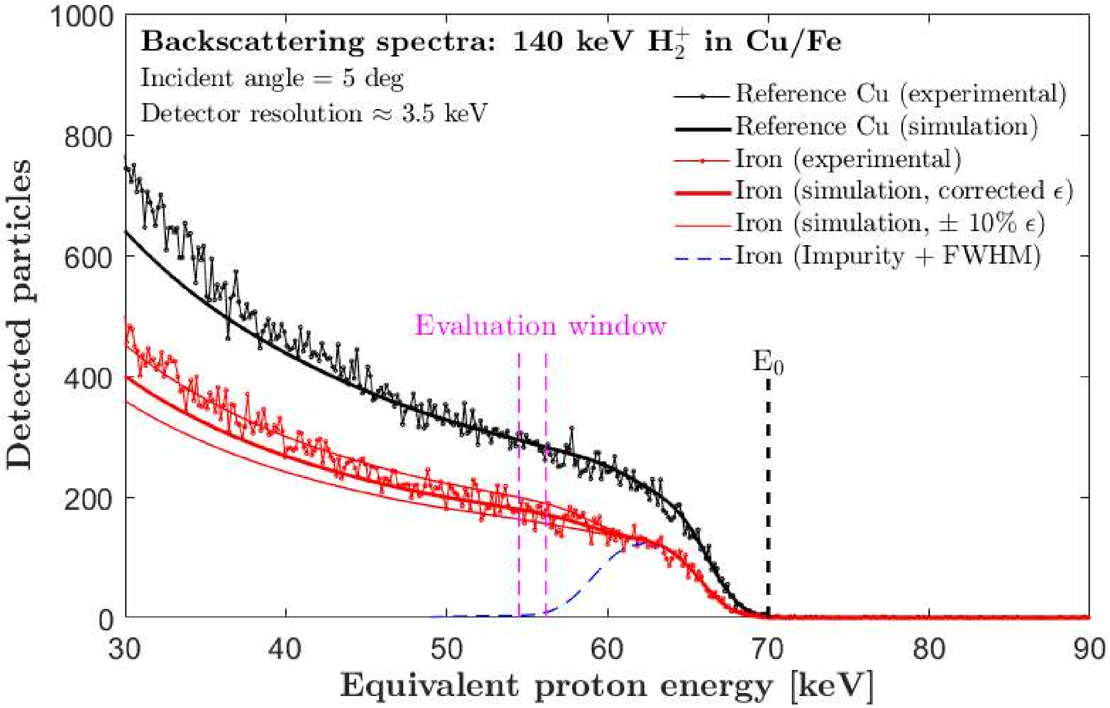




S. A. Correa, E. Pitthan, M. V. Moro, D. Primetzhofer, *Nucl. Instr. Meth. Phys. Res. B,* **478,** 104 (2020).

Electronic Stopping Power

Evaluation procedure



Incident particles x solid angle product

Detector efficiency x channel gain

$$H_{Fe} = \left[\frac{N_0 \Delta\Omega}{\cos\alpha}\right] \frac{\eta \in}{[\varepsilon_{Fe}]_0} \left(\frac{d\sigma}{d\Omega}\right)_{Fe}$$

Incident angle

Scattering cross-section

$$\frac{H_{Fe,exp}}{H_{Cu,exp}} = \frac{(d\sigma/d\Omega)_{Fe,exp}}{(d\sigma/d\Omega)_{Cu,exp}} \frac{[\varepsilon_{Cu,exp}]_0}{[\varepsilon_{Fe,exp}]_0}$$

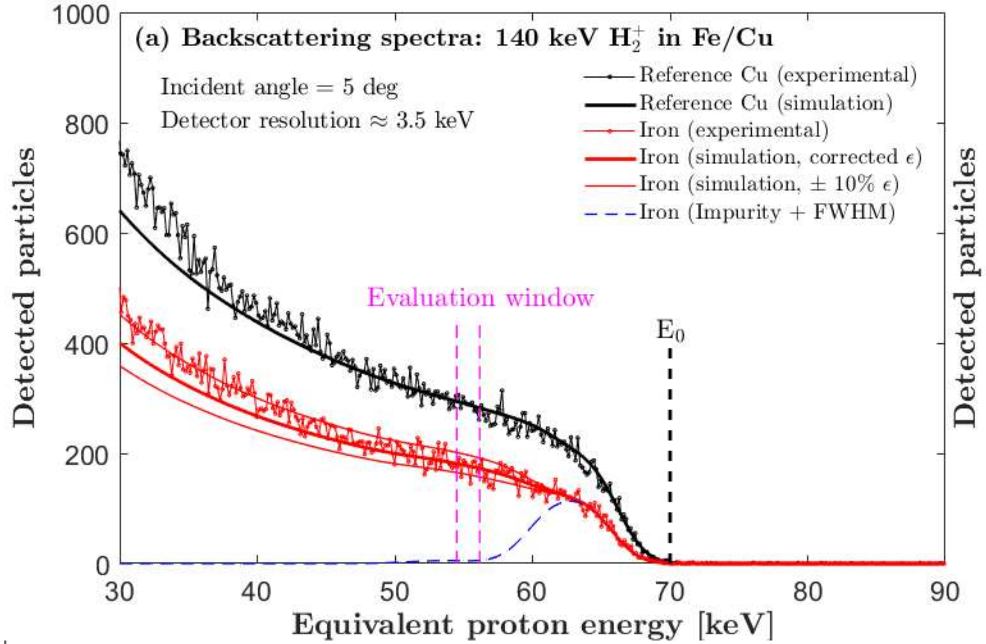
$$[\varepsilon_{Fe,exp}] = \sum_{Emin}^{Emax} \left(\frac{H_{Cu,exp}/H_{Cu,sim}}{H_{Fe,exp}/H_{Fe,sim}}\right) [\varepsilon_{Cu,exp}] \frac{[\varepsilon_{Fe,sim}]}{[\varepsilon_{Cu,sim}]}$$

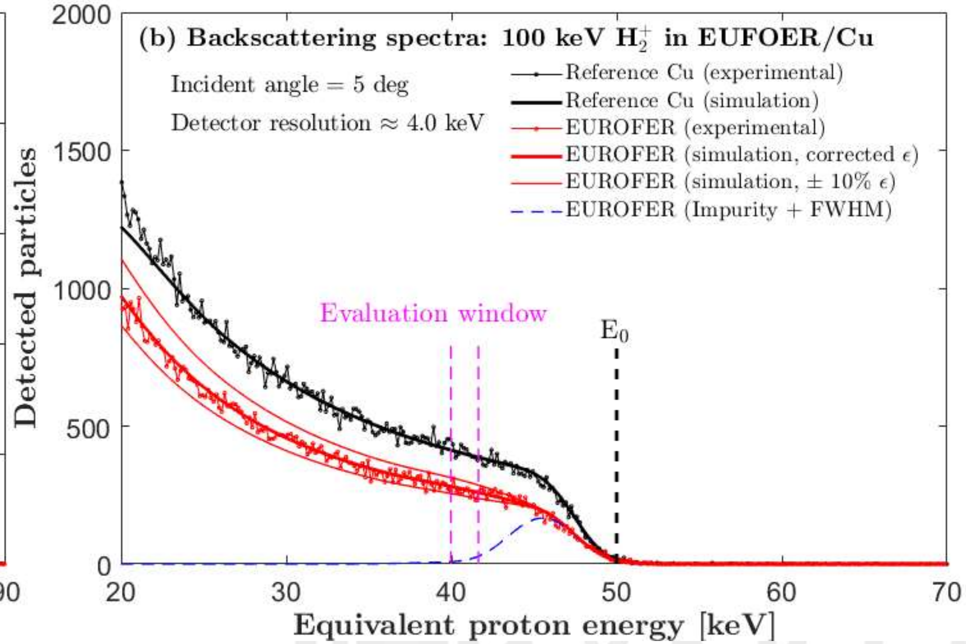
M. V. Moro et al., *Phys. Rev. A* **102** (2020)
M. V. Moro et al., Nucl. Instrum. Meth B **498** (2021)

Electronic Stopping Power

Stopping data for Fe & EUROFER in the medium/low energy regime

Experimental procedure

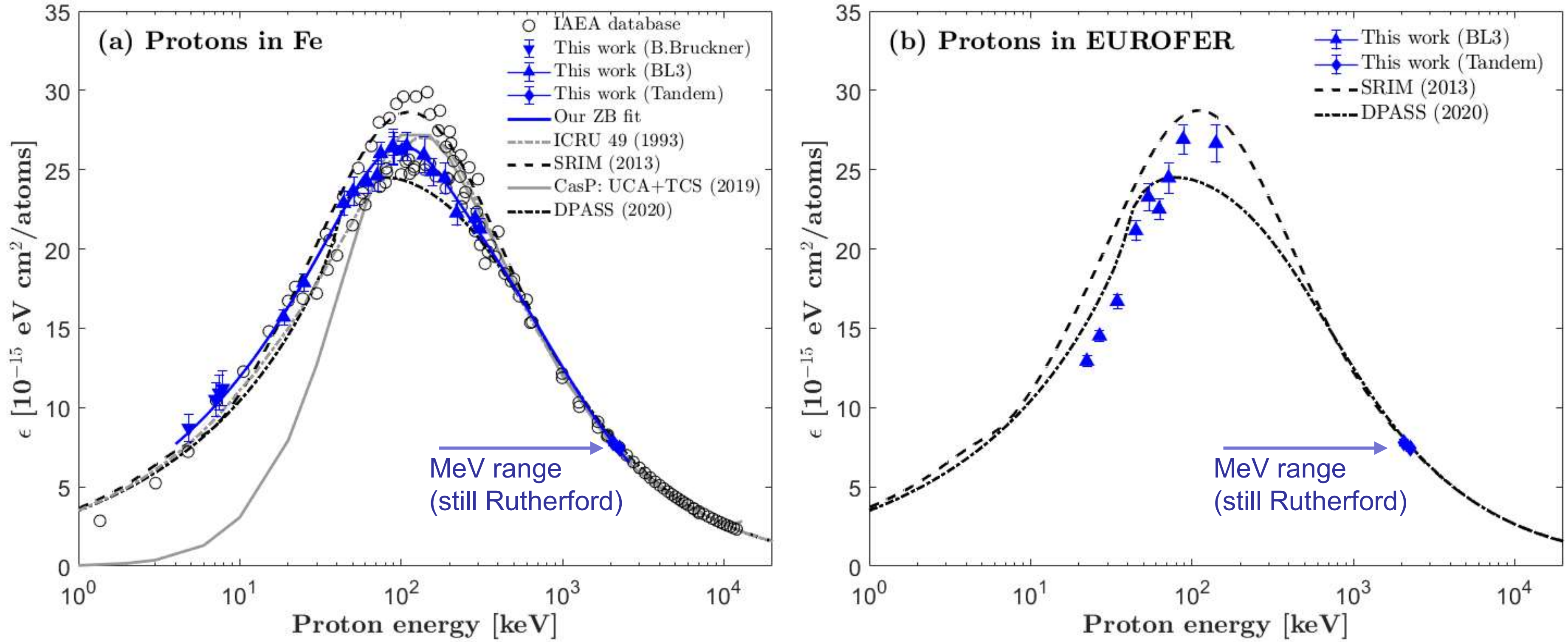




Electronic Stopping Power

Stopping data for Fe & EUROFER in the medium/low energy regime

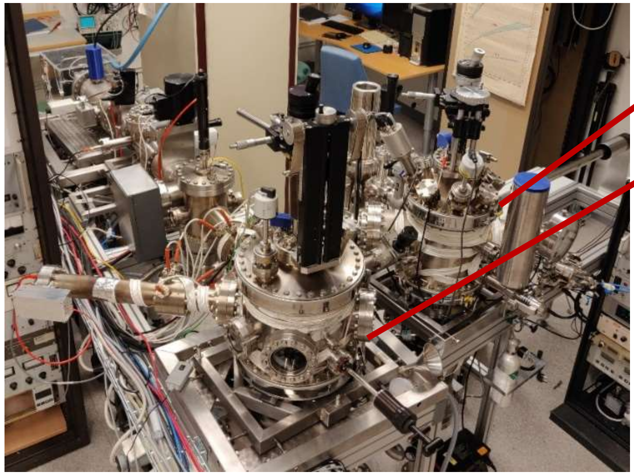
Experimental results



Electronic Stopping Power

Stopping data for Fe & EUROFER in the medium/low energy regime

Next steps: low energy regime ($E_0 \leq 10$ keV) [PhD student: Jila Shams]

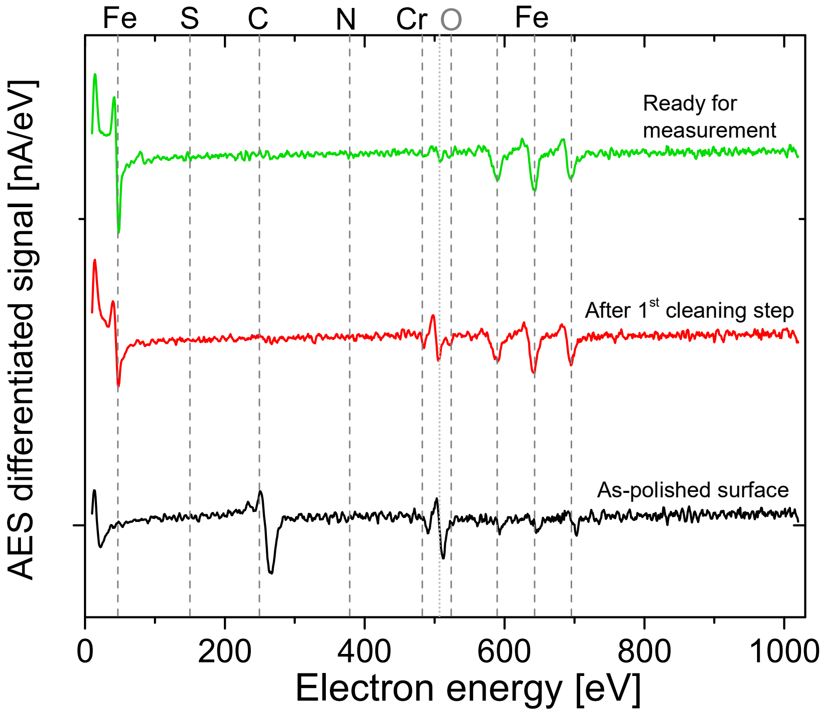


M. Draxler et al. Vacuum, **73** (2004).

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

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

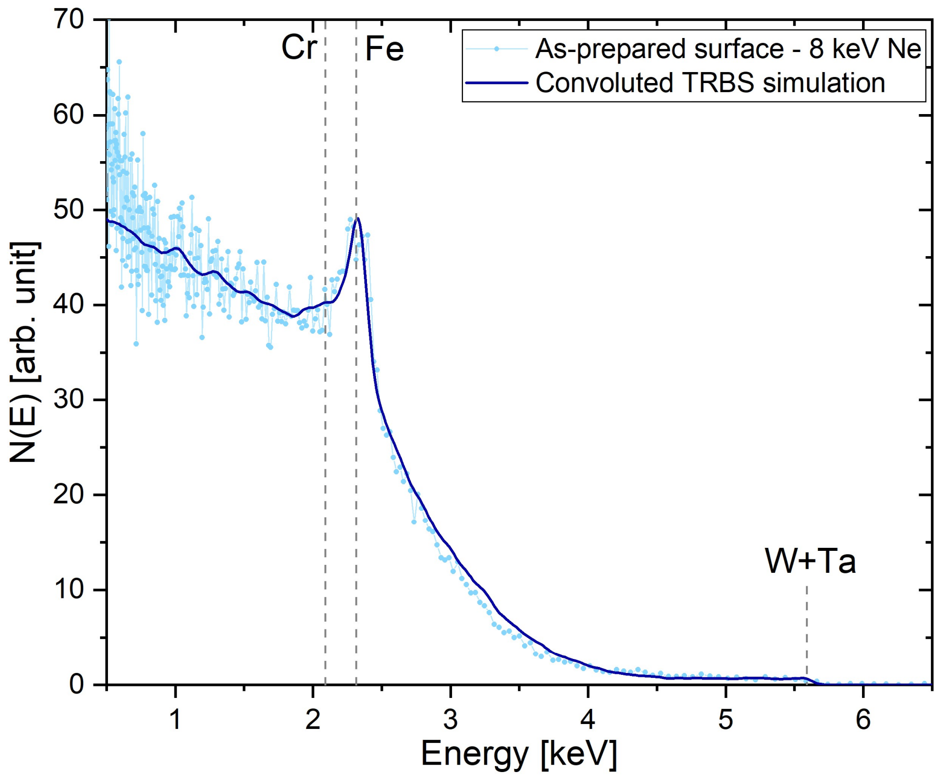
EUROFER cleaning cycle:
Argon sputtering/Annealing (300° C)

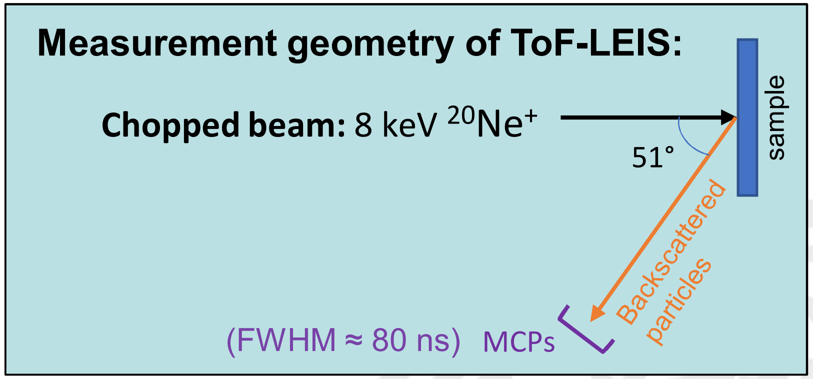


Electronic Stopping Power

Stopping data for Fe & EUROFER in the medium/low energy regime

Next steps: low energy regime ($E_0 \leq 10$ keV) [PhD student: Jila Shams]





- Energy converted ToF-LEIS spectrum from as-prepared surface of EUROFER97 sample (after polishing and in-situ cleaning procedures) using 8 keV Ne projectiles with the scattering angle of 129°.

- Composition according to MC simulations (TRBS):

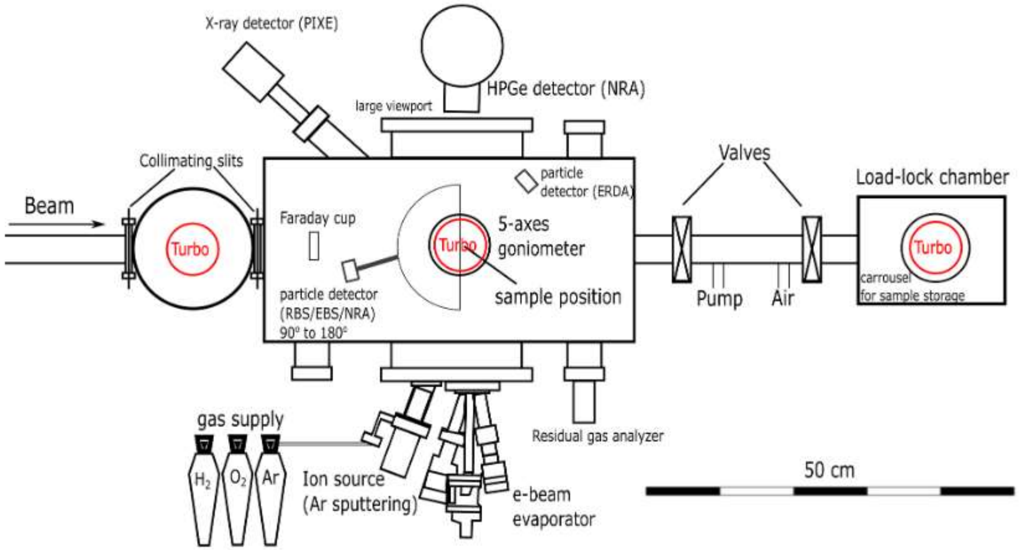
Layer 1: 10 Å, d=5.187 g/cm³, Fe= 46.6 at%, Cr= 5.0 at%, W= 0.42 at%, O= 48 at%
Layer 2: 20 Å, d=5.455 g/cm³, Fe= 50.2 at%, Cr= 5.0 at%, W= 0.80 at%, O= 44 at%
Bulk: 200 Å, d=7.846 g/cm³, Fe= 89.3 at%, Cr= 10.2 at%, W= 0.42 at%

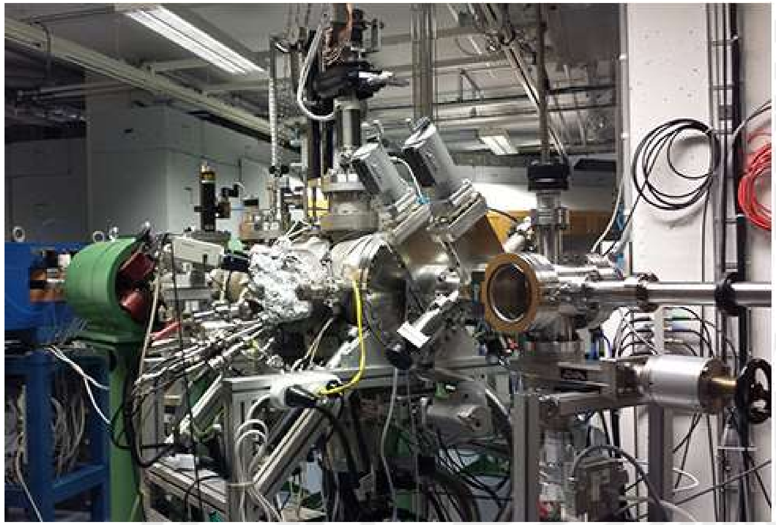
Working-packages

Sputtering yields and BCA simulations

- **Working-package 5 (W-P 5) main deliverables/milestones for 2021:**

→ QCM set-up assembling at UU.





Allows *in-situ* implantation/erosion investigations simultaneous to material characterization by IBA

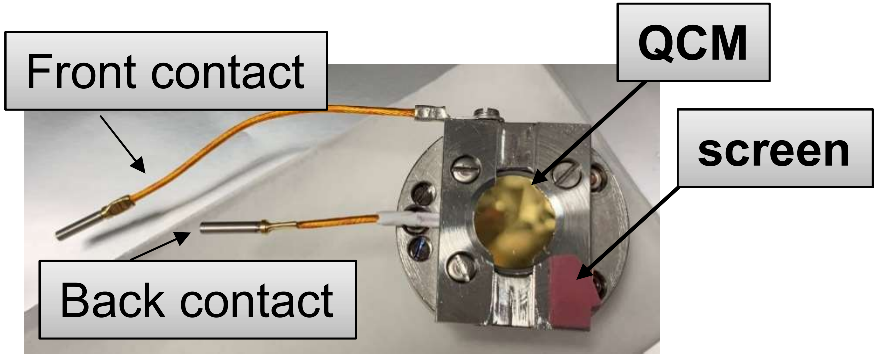
K. Kantre, M. V. Moro, *et al*. *Nucl. Instr. Meth. Phys. Res. B,* **463,** 96 (2020).

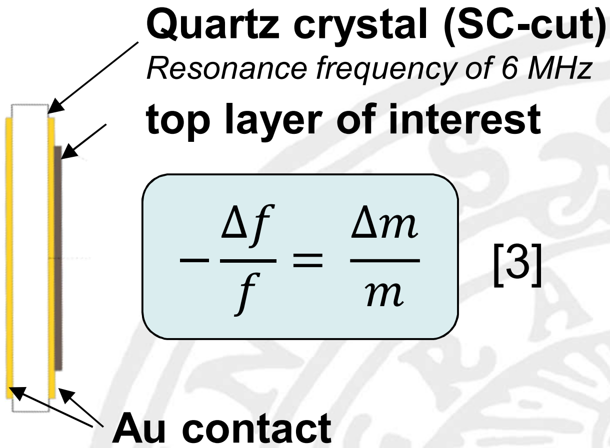
Sputtering yields

QCM set-up assembling at UU

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).

[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)

Working-packages

Ion irradiation experiments

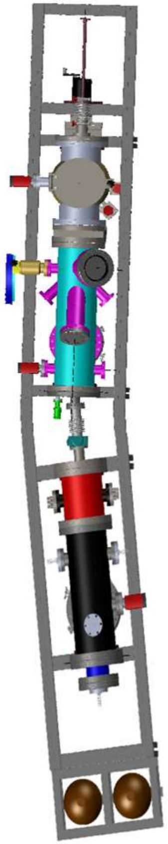
Low-Energy Ion Implanter (1 eV – 10 keV)

- **Working-package 6 (W-P 6) main deliverables/milestones for 2021:**

→ Define irradiation conditions: ions, energy, fluencies within different (ex-situ and in-situ) set-ups.

Energy: 0.5-4 keV, D_2^+.
Fluence ≈ 1×10^{22} D/m^2.

→ **Ex-situ:** Dedicated low-energy ion implanter.



Working-packages

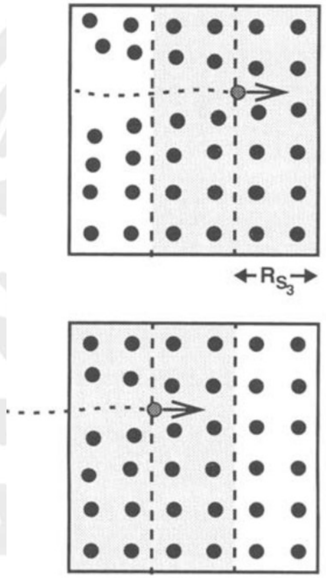
TD-DFT and Molecular dynamics

Working-package 7 (W-P 7) main deliverables/milestones for 2021:

→ MDRANGE simulations of ion implantation ranges and sputtering yields from surfaces with evolving composition. (A. E. Sand, Aalto University, Finland).

- Changed schedule: begun MD simulations of sputtering (D7.4) with existing MD model, in response to TU Wien's preliminary QCM measurements showing unexpected results compared to SDTrimSP (reported in September meeting).
- Investigating angular dependence and dependence on surface morphology
- Status of TD-DFT: expected to start in January 2022.

- Principle of **MDRANGE**: efficient ion range calculation by considering only recoil and small region of target in MD framework.



Working-packages

TD-DFT and Molecular dynamics

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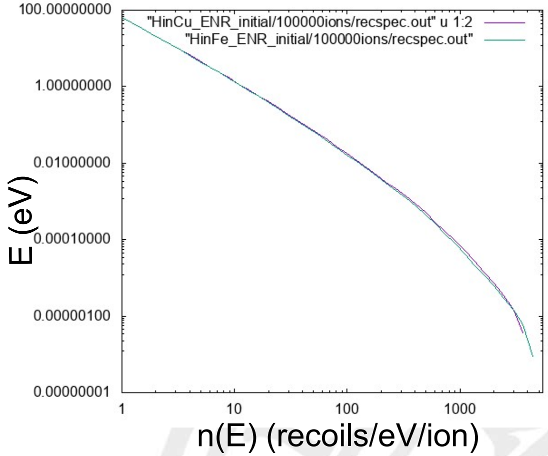
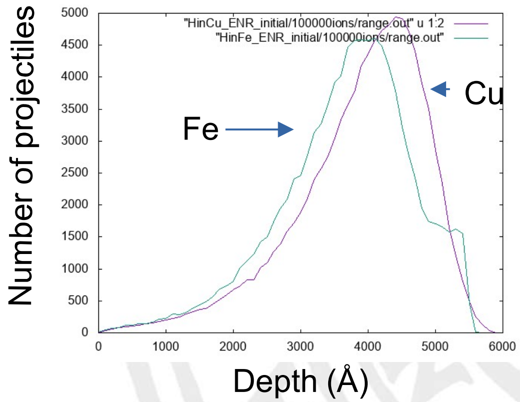
❑ Working-package 7 (W-P 7) main deliverables/milestones for 2021:

→ MDRANGE simulations of ion implantation ranges and sputtering yields from surfaces with evolving composition. (A. E. Sand, Aalto University, Finland).

- Preliminary calculation with existing model in **MDRANGE**:
  - H ions (70 keV) in Fe and Cu (for comparison to experimental work at UU)
  - < 1% are backscattered
- *Next steps: code development to get angles of scattered ions, implement selective output to facilitate better statistics.*





Achievement of Scientific Deliverables (2021)

- **Completed:**

→ IBA characterization of pristine materials (W, Fe, and EUROFER).
→ Stopping power of pristine PFCs samples in medium range:
  → Fe: from 4 to 330 keV for protons (up to 2 MeV).
  → W: 20 to 6000 keV for protons and 50 to 9000 keV for helium.
→ QCM installation in UU set-up.

- **In Progress:**

→ EUROFER: from 20 to 330 keV for H and He.
→ Sample characterization/preparation in the low-energy experimental system.
→ Stopping power in the low of pristine PFCs samples in low energy range.
→ Sputter yields D_2 on PFCs samples.
→ Theoretical calculation of electronic stopping power of light ions in pristine W, Fe and Fe-alloys using TD-DFT calculations.

Activities foreseen for 2022

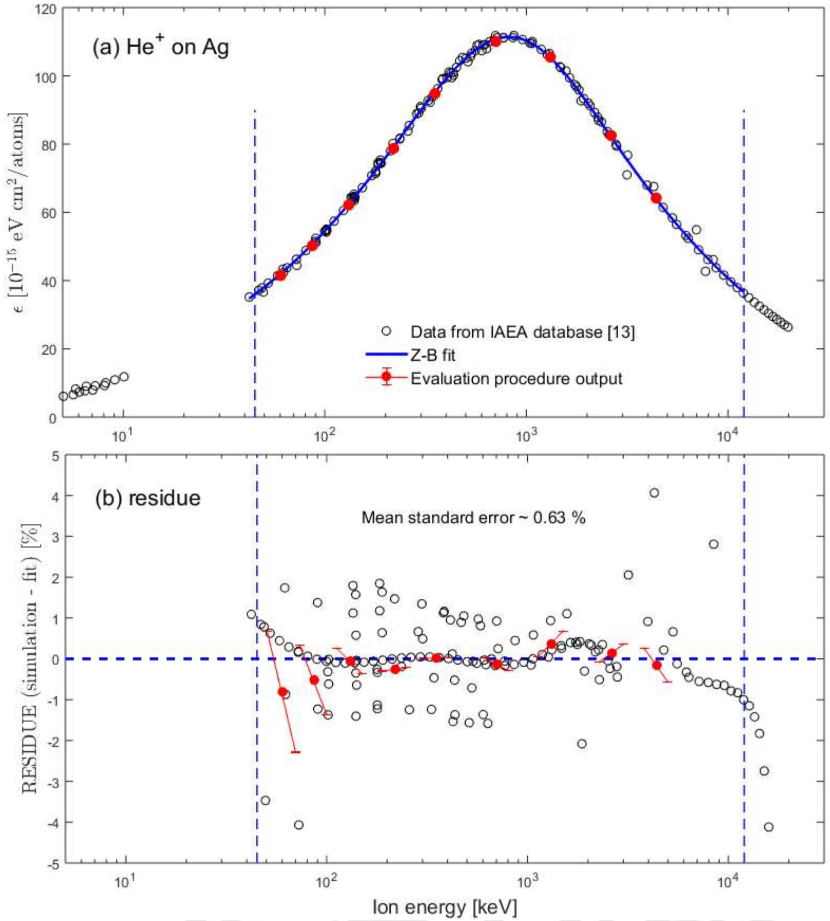
- Characterize damaged samples and continue monitoring pristine samples for quality control.
- Stopping power of pristine PFCs samples for light ions (sub-keV regime).
- In-situ preparation of the pristine crystalline Fe and W samples for ToF-LEIS/MEIS and angular scans.
- Sputtering yields and angular distributions of pristine W and EUROFER97 samples.
- Ex-situ ion irradiation experiments on the PFCs samples at UU.
- Theoretical calculation of electronic stopping power for random trajectories of light ions in pristine W, Fe and Fe-alloys using TD-DFT calculations.

EXTRAS

Electronic Stopping Power

Reference stopping data: Cupper

- Reference data for e.g., Cupper:
  - a) Data points: +250 H^+ and +100 for He^+
  - b) Statistical uncertainties < 3%
  - c) Traceable uncertainties (absolute meas.)
  - d) Data sets after 1990
  - e) Including complementary methods between P. Bauer and P. Mertens (different groups, set-ups, etc)
- Evaluation procedure / Different interpolations
- Different samples
- Good agreement in a wide energy range



1. D. Roth et al., *Phys. Rev. Letters* **118** (2017)
2. M. V. Moro et al., *Nucl. Instrum. Meth. B* **424** (2018)
3. M. V. Moro et al., *Phys. Rev. A* **102** (2020)
4. M. V. Moro et al., Nucl. Instrum. Meth B **498** (2021)

Low energy potentials

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

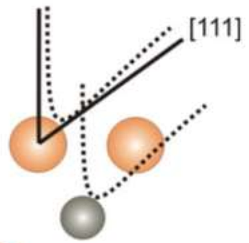
$$V(r) = \frac{Z_1 Z_2 e^2}{r} . \Phi(\frac{r}{a})$$

Screening function (Φ)

Screening lenght (a)

$$a = c_a a_f$$

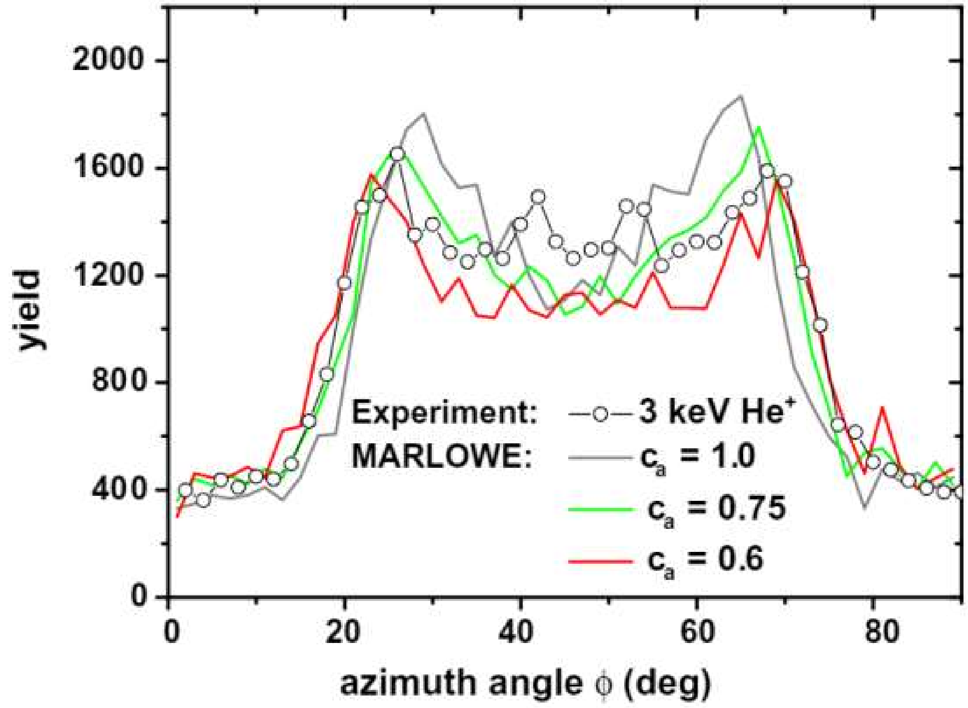
Correction factor (empirical) (c_a)



In-plane atoms

Out-of-plane atoms

Sample: Cu(100); **α =** 0 deg



D. Primetzhofer et al. / Surface Science 602 (2008) 2921–2926

For a given θ:

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