Detection of DEfects and HYDROgen by ion beam analysis in Channelling mode for fusion – DeHydroC

Project code: ENR-MAT-01-JSI

Mid-term report on research activities in 2021 and 2022
28. September 2022

Sabina Markelj (PI) on behalf of the team

Jožef Stefan Institute

MAX-PLANCK-INSTITUT FÜR PLASMAPHYSIK

cea

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Team members

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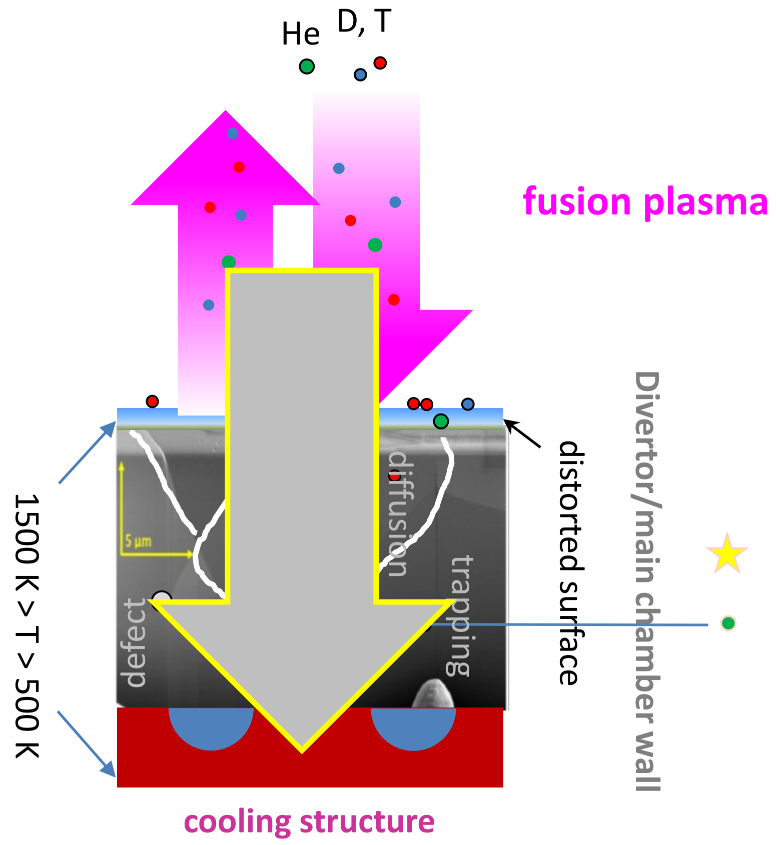
Motivation

Simplified fusion device scenario

Tungsten –plasma facing material

$10^{24} m^{-2}s^{-1} > j > 10^{18} m^{-2}s^{-1}$

eV < E < keV



- neutron damage – 5 dpa/fpy [1]
- He production

[1] Federici et al., Nucl. Fusion 57 092002, 2017

Motivation

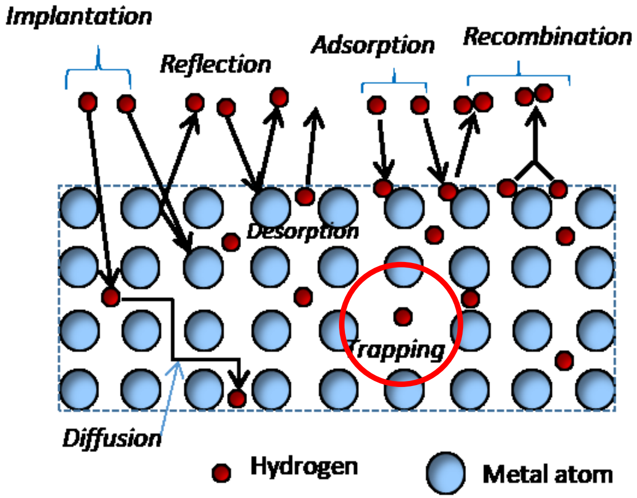
Simplified fusion device scenario

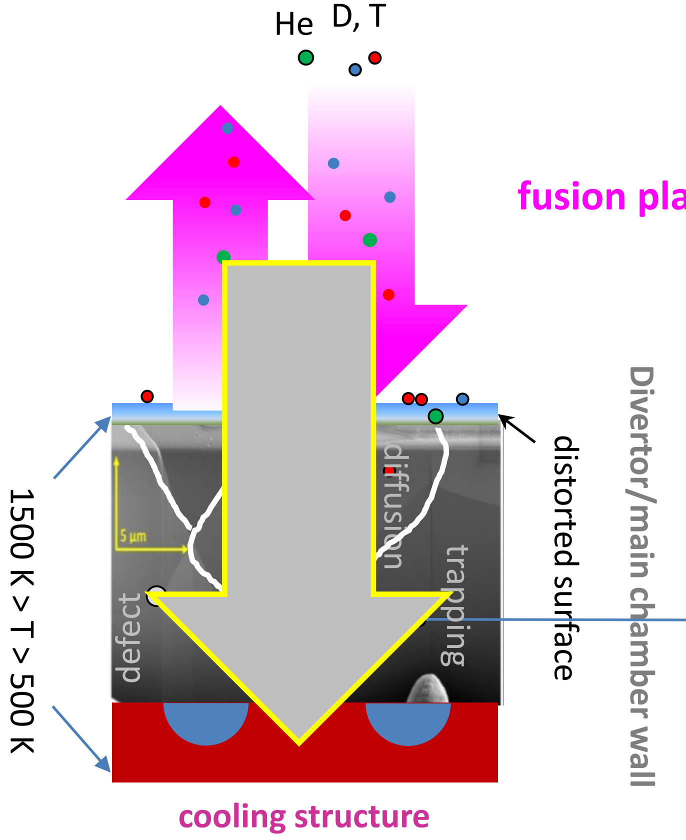
Tungsten – plasma facing material

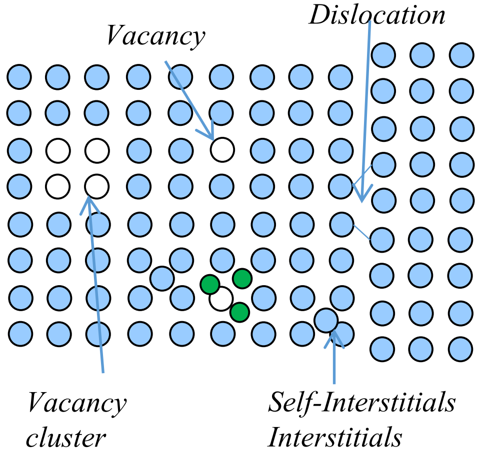
$10^{24} m^{-2}s^{-1} > j > 10^{18} m^{-2}s^{-1}$

eV < E < keV

Displacement damage creation
- Material properties change







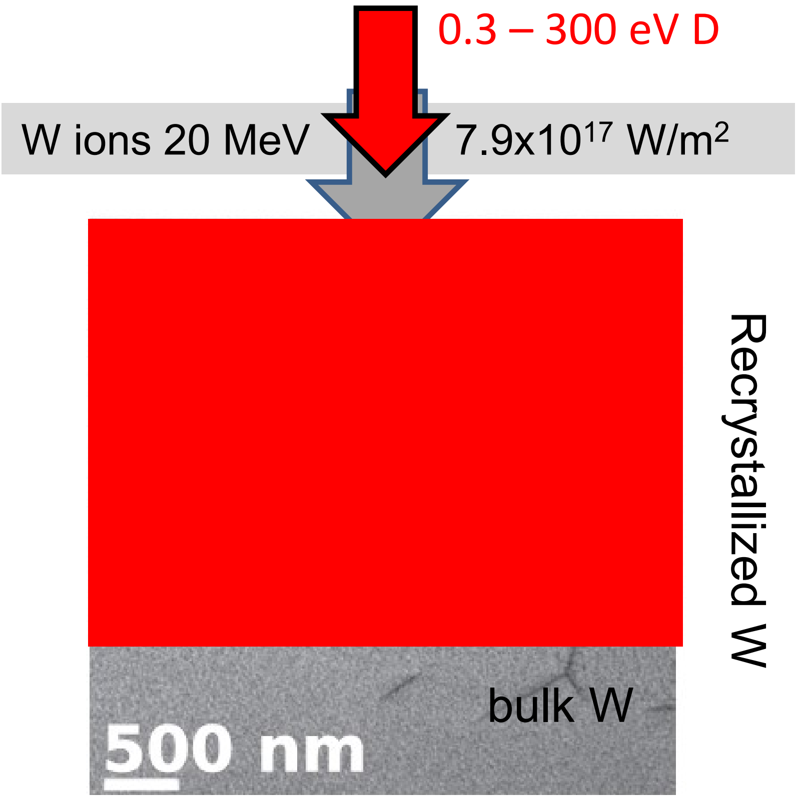
neutron damage – 5 dpa/fpy [1]

He production

[1] Federici et al., Nucl. Fusion 57 092002, 2017

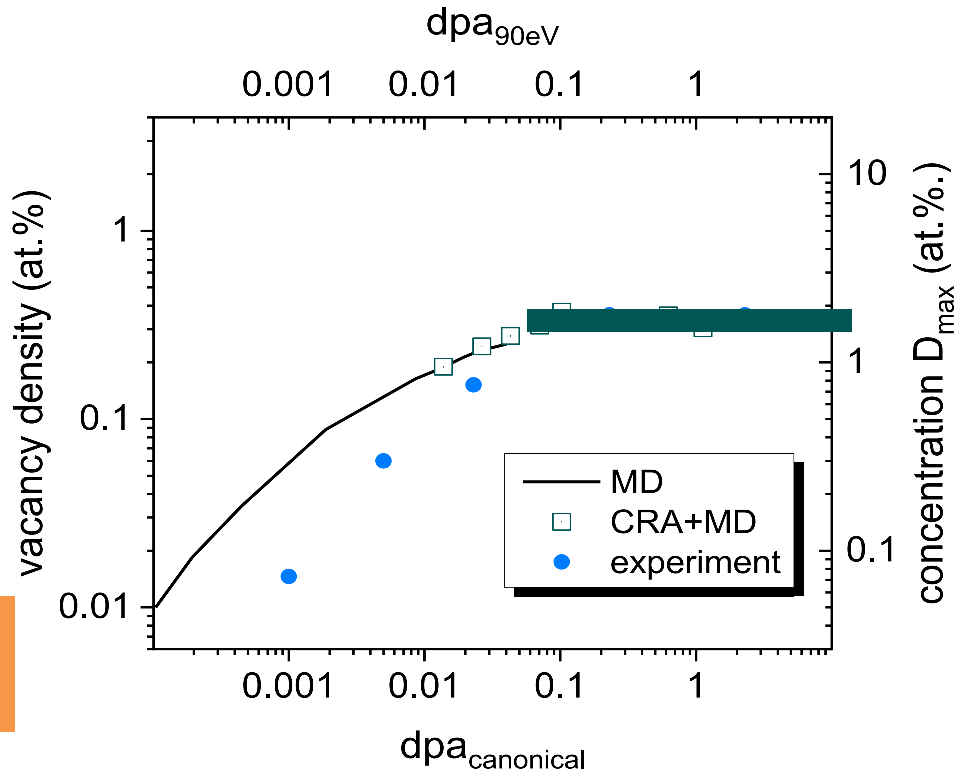
D retention analysis versus defect concentration

Hydrogen isotopes are trapped in defects created by i.e. high energy ion irradiation, neutron irradiation



STEM on
FIB lamela

No displacement damage –
D retention 10^{-3} at. %



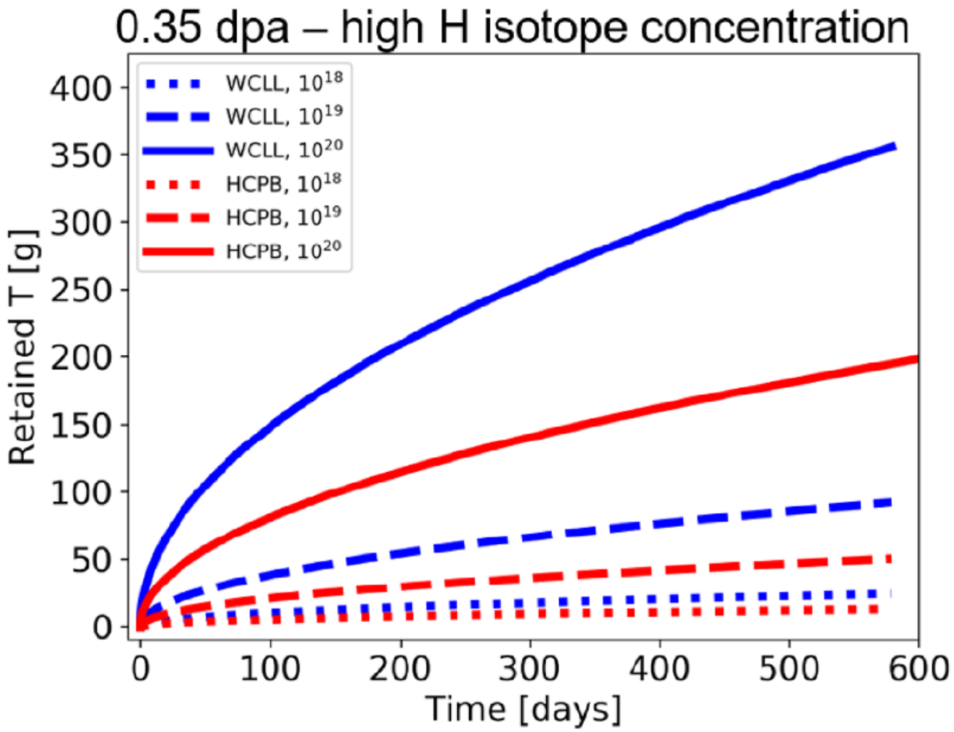
MD modelling of defect creation in hydrogen-free tungsten compared to measured D concentration *[Mason et al. Phys. Rev. Mat. 5 (2021) 095403]*

Methodology to quantify defect evolution and defect concentration

- ➢ measure D concentration by nuclear reaction analysis (NRA) and desorption kinetics by thermal desorption spectroscopy (TDS)

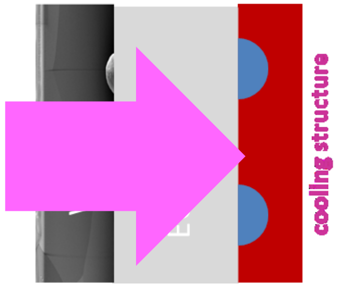
T. Schwarz-Selinger, ICFRM 2021

Tritium retention in DEMO



Arredondo et al. *Nuclear Materials and Energy 28 (2021) 101039.*

- First modelling of tritium permeation and retention in W for DEMO first wall



- Calculation based on experimental studies of simultaneous W ion damaging and D ion exposure by Markelj et al. NF (2019), Pečovnik et al. NF (2020) –

⇒ **Significant T retention**

⇒ **No steady state permeation flux within blanket lifetime**

- Applicable for DEMO? – need for microscopic understanding

- **Which are the defect types responsible for tritium retention and how they evolve at high temperatures?**

The DeHydroC project

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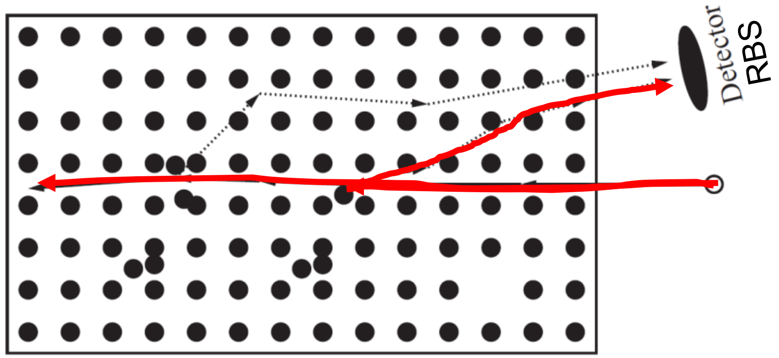
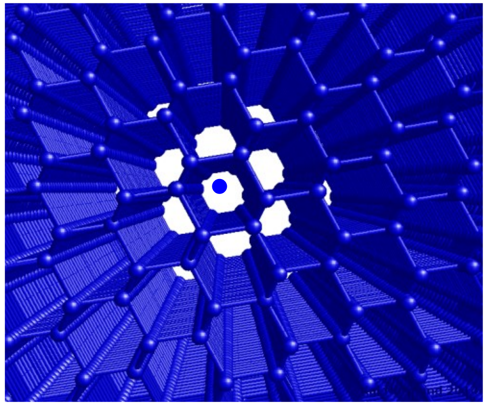
RBS channeling

Channeling Rutherford Backscattering Spectroscopy (C-RBS) is a well known method to measure disorder in materials due to ion irradiation – derive information of point defect distribution

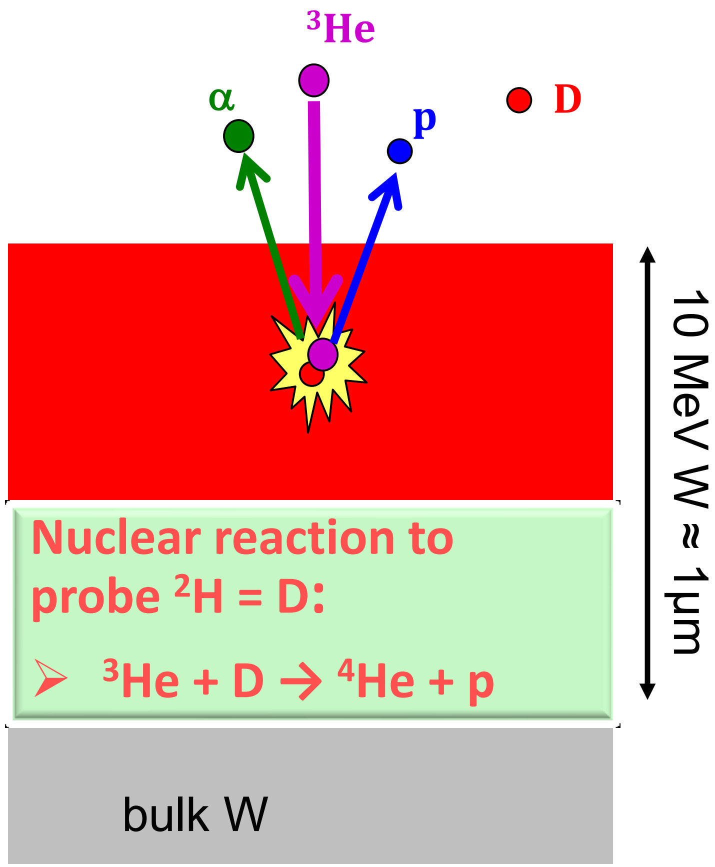


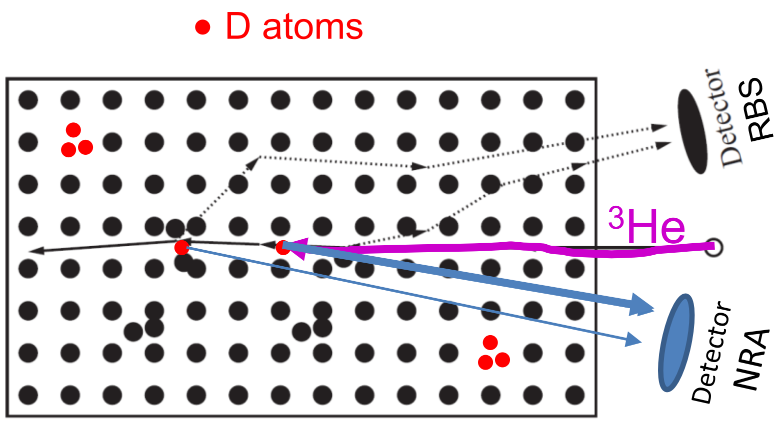


- Identify defects in displacement damaged tungsten by C-RBS with help of microstructure analysis methods by:
  - Electron Microscopy (SEM, TEM, STEM, …..)
  - Positron Spectroscopy (PALS, DB-PAS)

Sensitive mainly to dislocation structure (loops, lines)

D retention analysis by nuclear reaction analysis (NRA)





Deuterium depth profiles - Analyzing protons from nuclear reaction $D(^3He,p)^4He$ at different ^3He energies from 700 keV up to 4.3 MeV

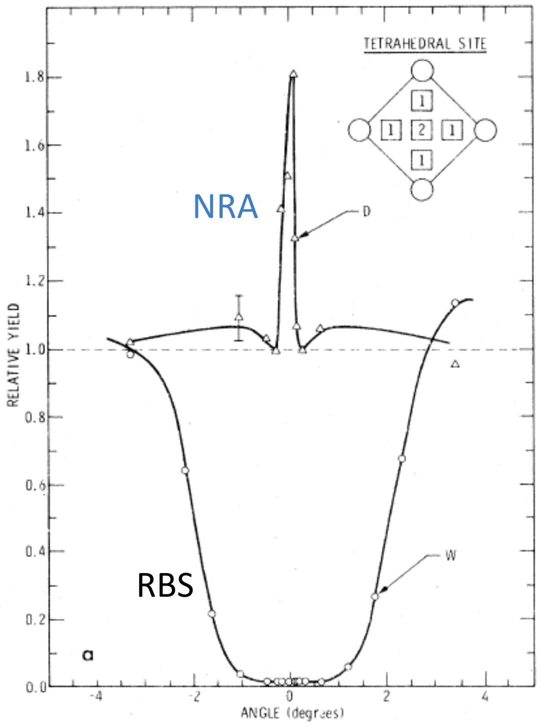
Deuterium trapped in open volume (vacancies, vacancy clusters, voids)

- C-RBS and C-NRA complementary for defect characterization

NRA channeling

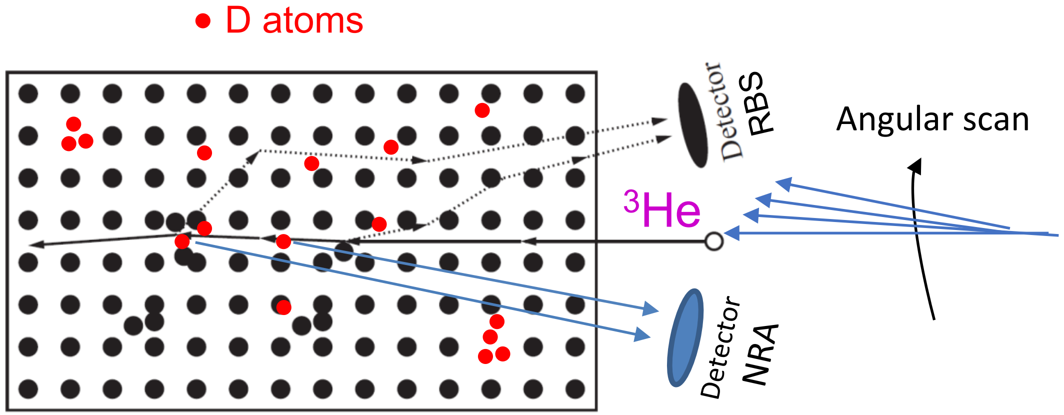
Method to determine hydrogen interstitial sites in metals in 70's/80's
[Fukai, The metal-hydrogen systems, Springer 2005]

- Examples of detection of hydrogen in metals by NRA-channeling



Angular scans through the <100> axis on W
Deuterium sitting in tetrahedral sites

Picraux, S. T. & Vook, F. L. Deuterium lattice location in Cr and W. Phys. Rev. Letters 33, 1216 (1974).



But:
- Academic case of defect free tungsten
- Only qualitative measure
- 30 keV D ions created vacancies by themselves, even possible to determined position of solute atoms, signal should be dominated by trapped D!

Goal of the project

The main goal of this project is to develop an experimental setup and analysis procedure (modelling code for spectra interpretation) that will enable detection of individual types of defects and the amount of hydrogen trapped in the defects.

- **Objective 1: differentiate defect structures in the channelling-RBS spectra: to separate small from large defects.**

- **Objective 2: perform NRA in channelling mode on a quantitative level to allow for determination of absolute deuterium amounts inside individual defects.**

- Create samples with one dominating defect type and decorate them with D
- Apply binary collision approximation (BCA) code RBSADEC recently developed at the UHEL [Zhang et al. Phys. Rev. E 94, 043319 (2016)] and further develop the modelling algorithm to identify defects from RBS-channeling and D position from NRA-channeling spectra
- Use TEM and PAS analysis to implement realistic defects into the code
- Development and application of an ion channelling set-up at the tandem accelerator laboratory in Ljubljana to characterize produced defects and D retention simultaneously.

- **Contribute to WP MAT-IREMEV and WP PWIE SP C**

DeHydroC project: 1. June 2021 – 31. May 2024

Work Package structure:

- **WP1 - The In-Situ Ion Beam Analysis in Channelling mode (INSIBA-C)**
  - **T1.1 Incorporation of the goniometer in the INSIBA experimental station – JSI.**
  - **T1.2 Detection system for ion beam methods - JSI.**
- **WP 2 - Sample production and defect characterization**
  - **Task 2.1 Production of samples with dominant defects in the material – JSI and MPG.**
  - **Task 2.2 Characterization of defects – University Helsinki (UHEL), JSI, MPG.**
  - **Task 2.3 Simulation and interpretation of C-RBS spectra - UHEL, CEA, JSI.**
  - **Task 2.4 In-situ C-RBS and sample heating – JSI, MPG, UHEL**
- **WP 3 - Deuterium retention studies**
  - **Task 3.1 Characterization of defects by D retention studies and MRE modelling - JSI, MPG, CEA, UHEL.**
  - **Task 3.2 Development of C-NRA method - JSI, UHEL, MPG.**
  - **Task 3.3 – Modelling of deuterium position in lattice/defect and identification of D position - UHEL, CEA, JSI.**
- **WP 4 - Management, Dissemination, Communication and Exploitation.**
  - **Task 4.1 Management.**
  - **Task 4.2 Dissemination, communication and exploitation**

DeHydroC project: 1. June 2021– 28. September 2022

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Activities till now

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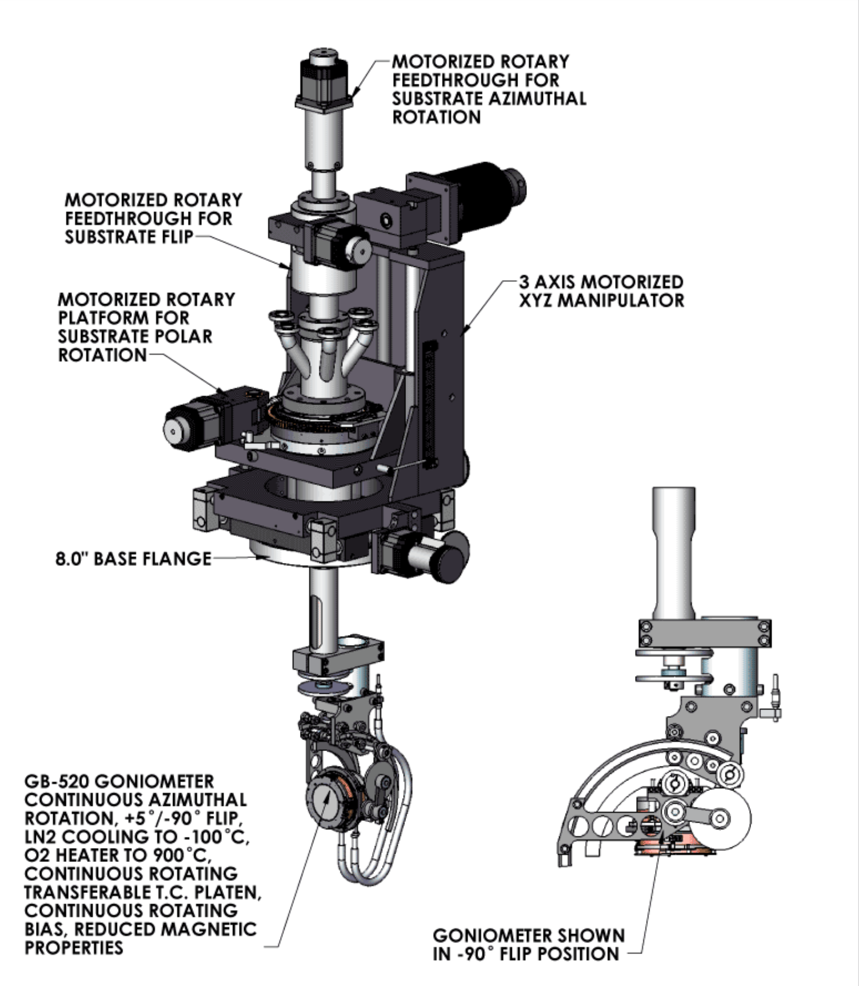
6-axis goniometer

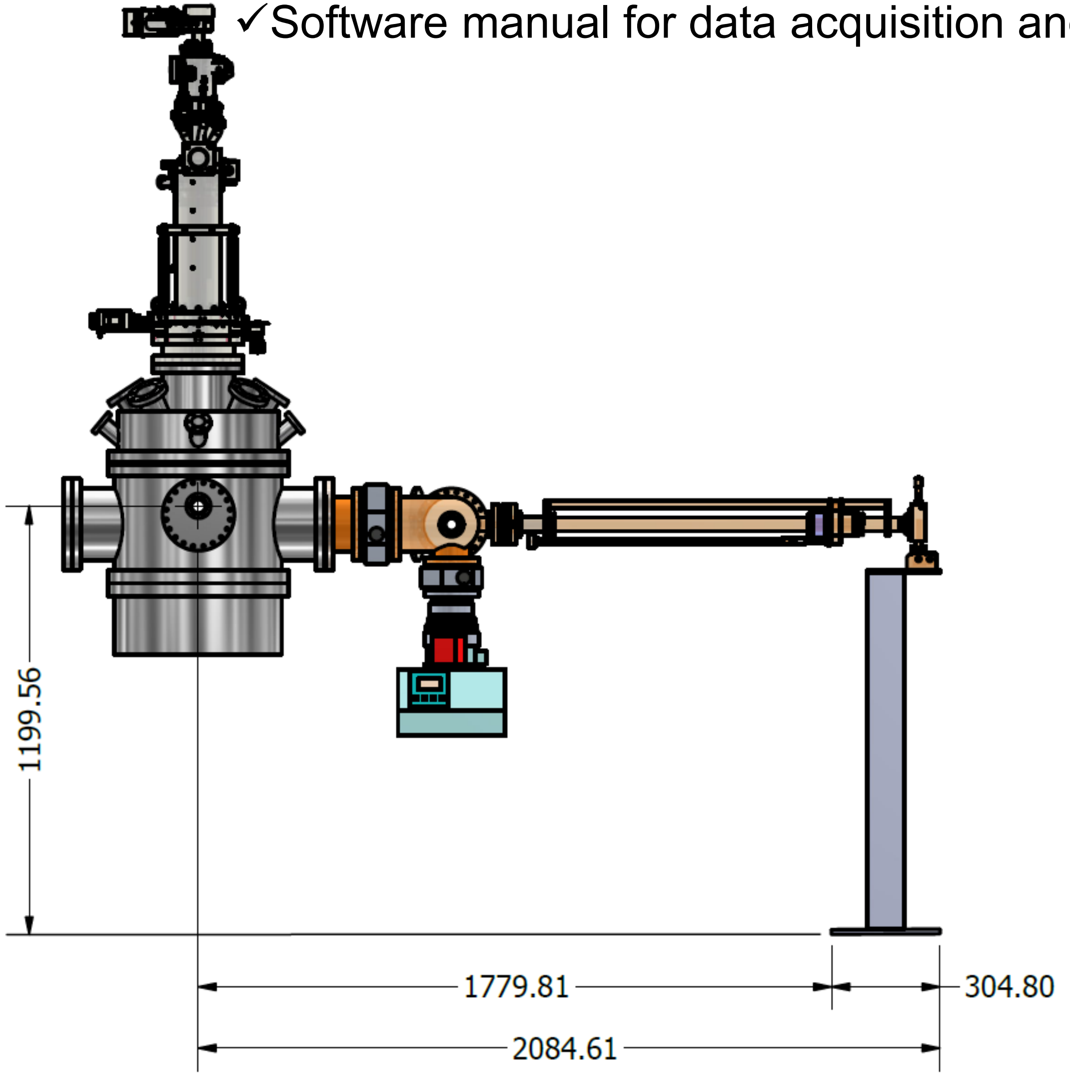
✓ JSI – 6-axis goniometer specified, public call, final order at National Electrostatic Corp. (NEC) 08/2021



Resolution in rotation: 0.01 degrees
Sample platen heating to 1200°C continuous
Liquid nitrogen cooling
Maximum sample bias 500 V
Sample size 4 cm
Data acquisition system for 5 detectors with computer and program for spectra collection
Additional: Load-lock chamber with magnetic arm

6-axis goniometer

- ✓ JSI – 6-axis goniometer specified, public call, final order at National Electrostatic Corp. (NEC) 08/2021, Planned delivery in October 2022 – delays due to Covid-19 and Ukraine war
  - ✓Software manual for data acquisition and goniometer



New cover for the vacuum chamber – produced

Activities in first half of the project

- **WP1 - The In-Situ Ion Beam Analysis in Channelling mode (INSIBA-C)**
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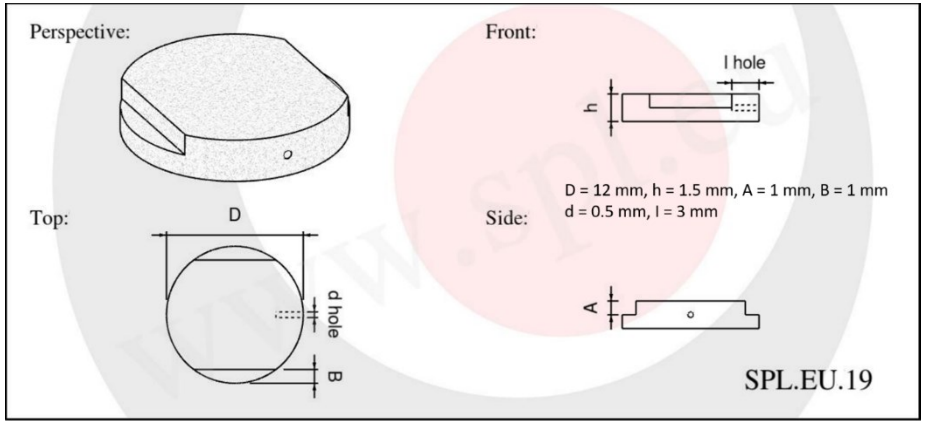
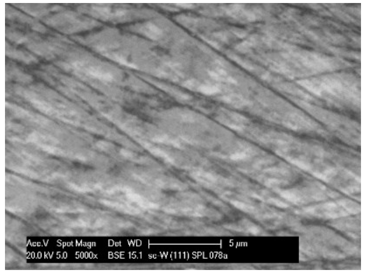
Single Crystal W (111) - Sample preparation

- W single crystal (111) – 9 samples, alignment < 0.4°, purchased at Surface Preparation Laboratory (SPL), Netherlands
- Sample design for easy handling, mounting, transfer

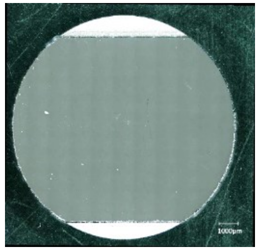


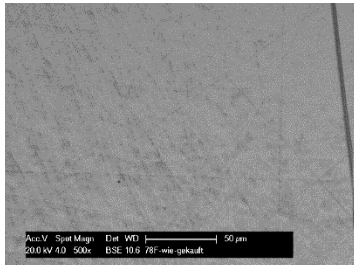
As delivered:

- Mirror polished surfaces
- But near surface distortions



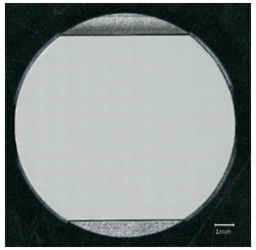
SEM

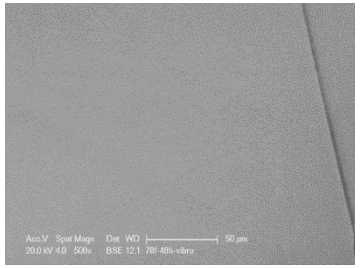




Additional sample treatment that was efficient and reproducible (IPP)
(checked by SEM and PALS):

- grinding, electropolishing, vibro-polishing
- Annealing at 2350 K in vacuum for 5 min





Initial plan for damaging – creation of single dominating defects in sample

DeHydroC goal, to make samples with one dominating defect type - different options

Light ions (200 keV D ions)

- Isolated cascades: vacancies?
- Effect of D?

Heavy ion W (10.8 MeV W ions)

- Denser cascades

Damage level

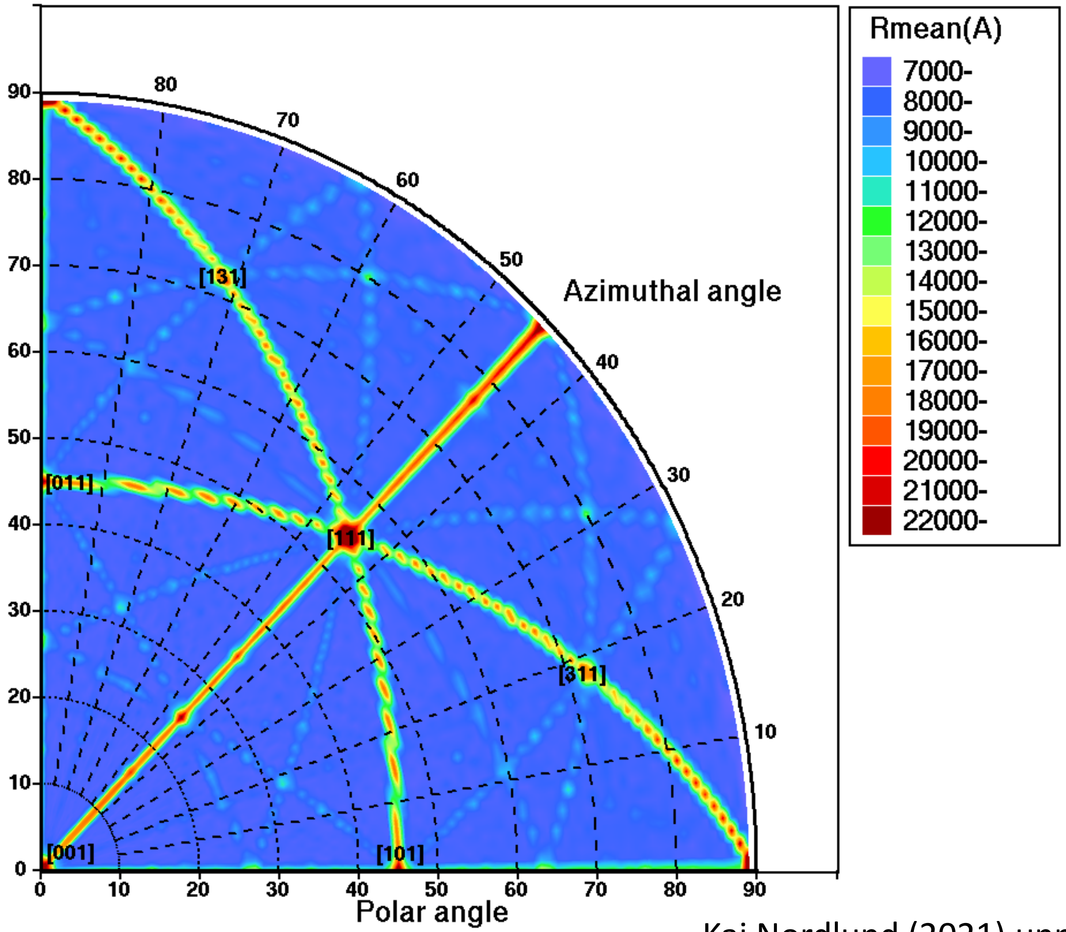
- 'High', to see something in C-RBS
- 'Low', to learn something from PAS

Temperatures

+ room temperature
+ 800 K

7 degrees rotated and tilted

Mean ion range of 10 MeV W ions on W by angle

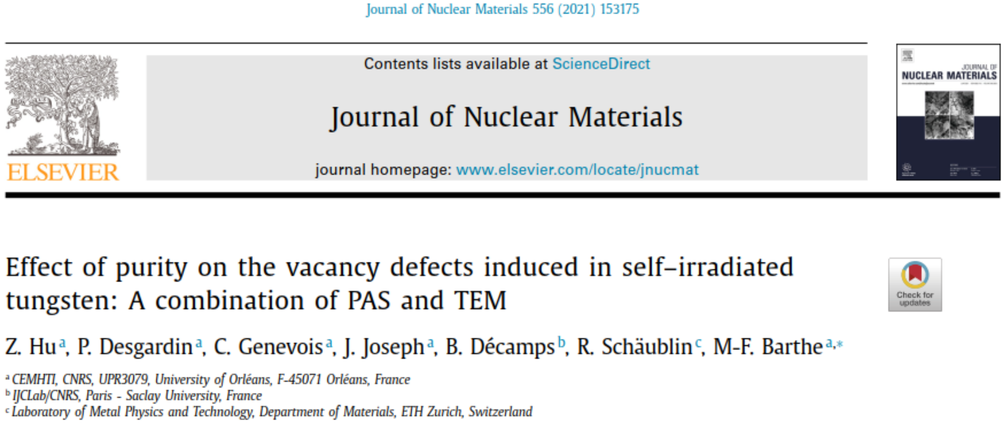


Kai Nordlund (2021) unpublished

Samples prepared

Decided to go with only 10.8 MeV W ion irradiation, according to recent publications [Hu et al. JNM 556 (2021) 153175]

- **Mainly single vacancies at room temperature**
- **Larger vacancy clusters at 773 K**


Journal of Nuclear Materials 556 (2021) 153175

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journal homepage: www.elsevier.com/locate/jnucmat

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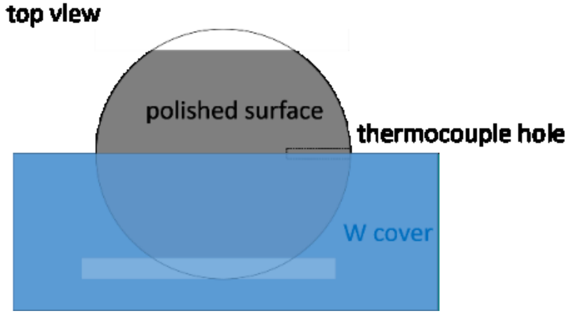
Effect of purity on the vacancy defects induced in self-irradiated tungsten: A combination of PAS and TEM

Z. Hu[a], P. Desgardin[a], C. Genevois[a], J. Joseph[a], B. Décamps[b], R. Schäublin[c], M-F. Barthe[a,*]

[a] CEMHTI, CNRS, UPR3079, University of Orléans, F-45071 Orléans, France
[b] IJCLab/CNRS, Paris - Saclay University, France
[c] Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland

✓ For RBS channeling in Madrid + TEM characterization (2021)

	ID	Definition
1)	78f	'Heavily damaged standard': 0.2dpa, 290K
2)	78b	'Big vacancy clusters': 0.2 dpa, 800 K
3)	78g	'Single vacancies': 0.02 dpa, 290 K, half covered
4)	78c	'Small vacancy clusters': 0.02 dpa, 800 K

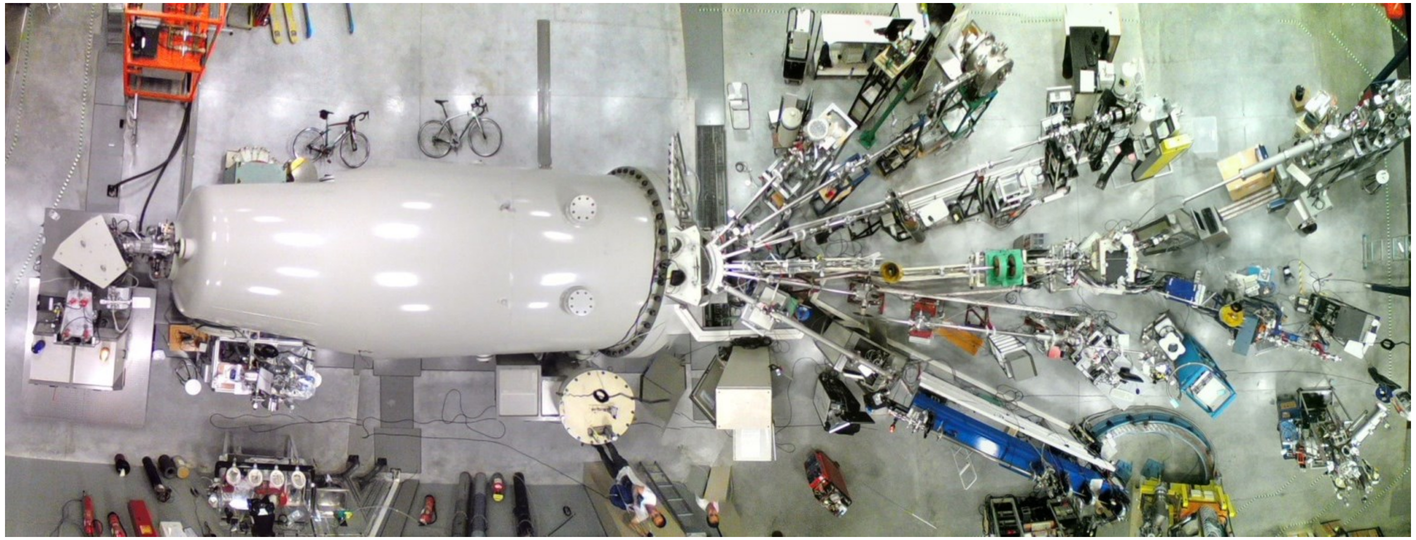


✓ For PAS/PALS analysis Helsinki (2022)

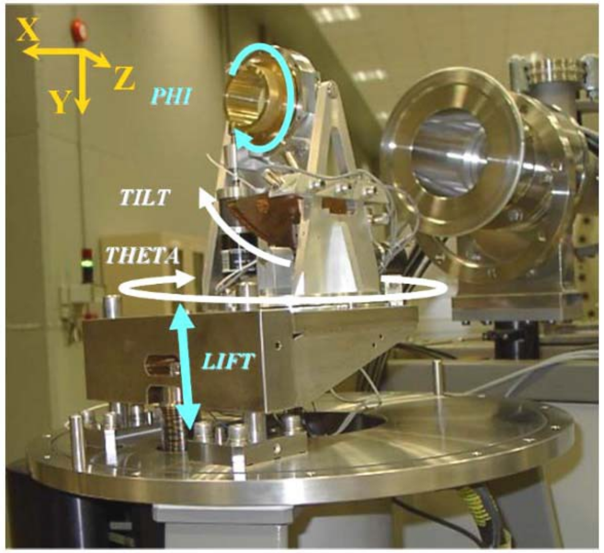
	ID	Definition
1)	78h	'Single vacancies': 0.02 dpa, 290 K
2)	78a	'Heavily damaged standard': 0.2dpa, 290K
3)	78e	'Big vacancy clusters': 0.2 dpa, 800 K
4)	78d	'Small vacancy clusters': 0.02 dpa, 800 K

Analysis of irradiated samples by C-RBS in Madrid

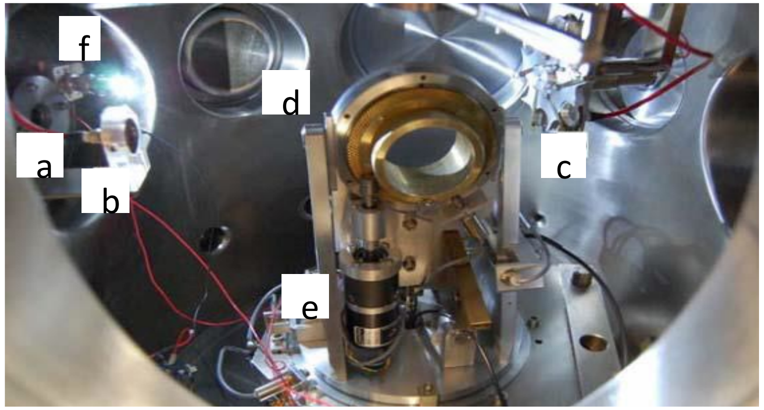
- JSI team visited *CMAM (Centre for Micro Analysis of Materials), UAM (Madrid.) for C-RBS measurements in September 2021*



5MV Accelerator Cockcroft-Walton (High Voltage Europe)

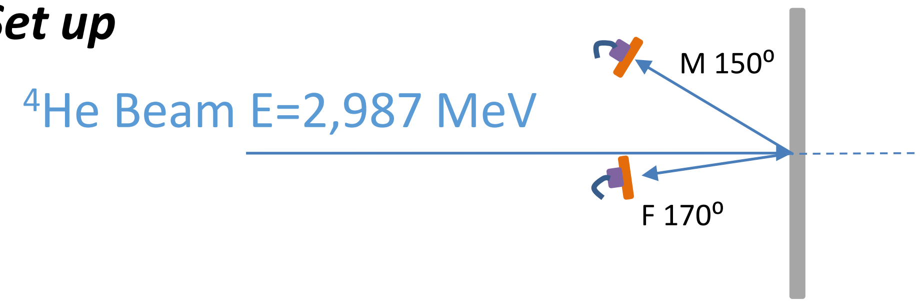


3 angles goniometer
(no heating)
(Panmure Instruments, UK)



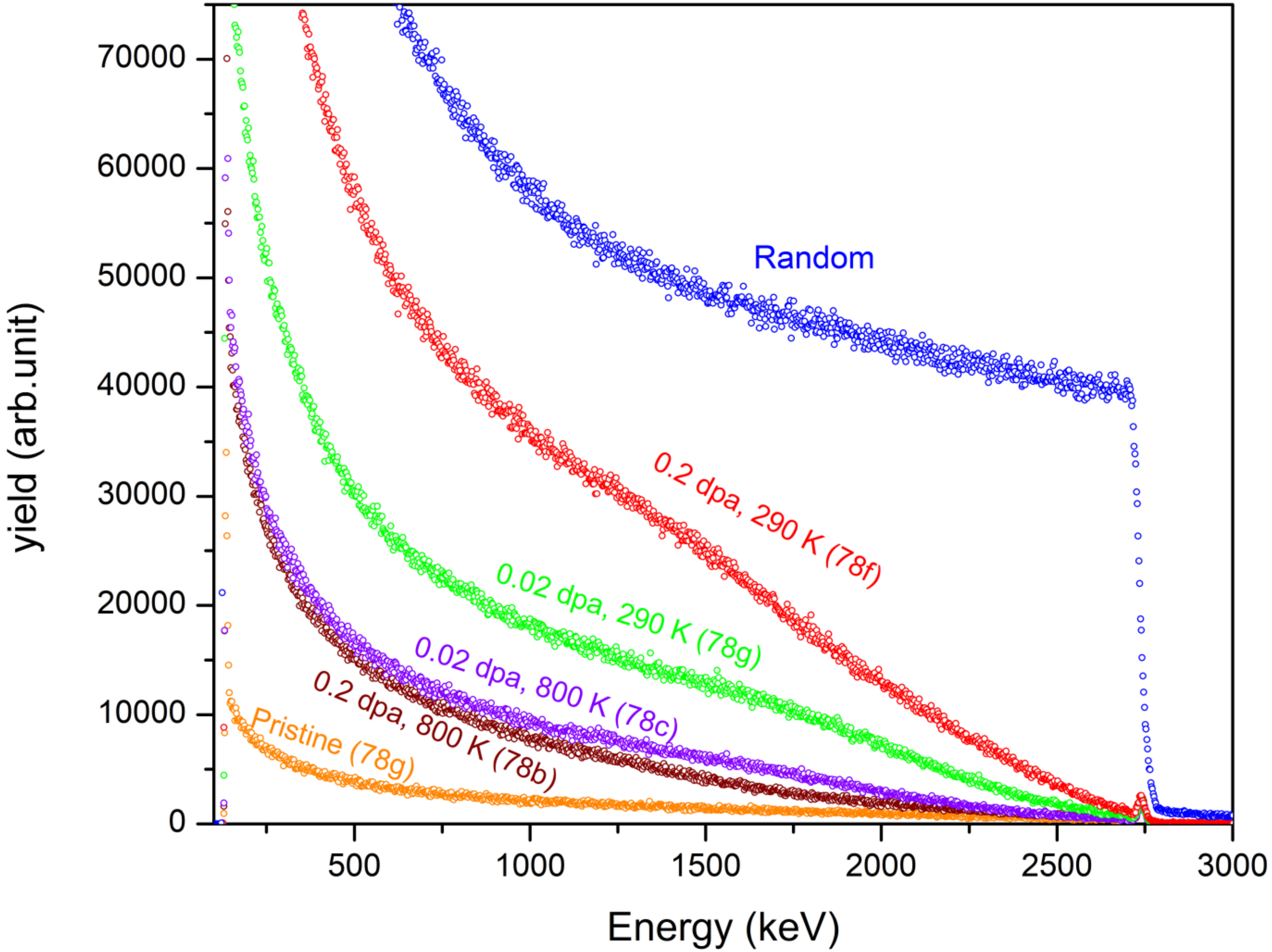
a: beam entrance
b: Si F detector
c: Si M detector
d: Ge detector (gamma)
e: goniometer
f: light

Set up



Analysis of irradiated samples by C-RBS – measurements

^{4}He beam E=2.987 MeV



Random = Σ100 spectra (5 µC)

<111> channelling direction

78f heavily damaged standard: 0.2dpa 290 K

78g single vacancies: 0.02 dpa 290 K

78c small vacancy clusters: 0.02 dpa 800 K

78b big vacancy clusters: 0.2 dpa 800 K

78g pristine

- ✓ Starting material (pristine sample) has a very good crystallinity
- ✓ We have observed differences between the irradiation damage treatments

Analysis of C-RBS spectra by RBSADEC simulation using randomly displaced atoms (RDA)

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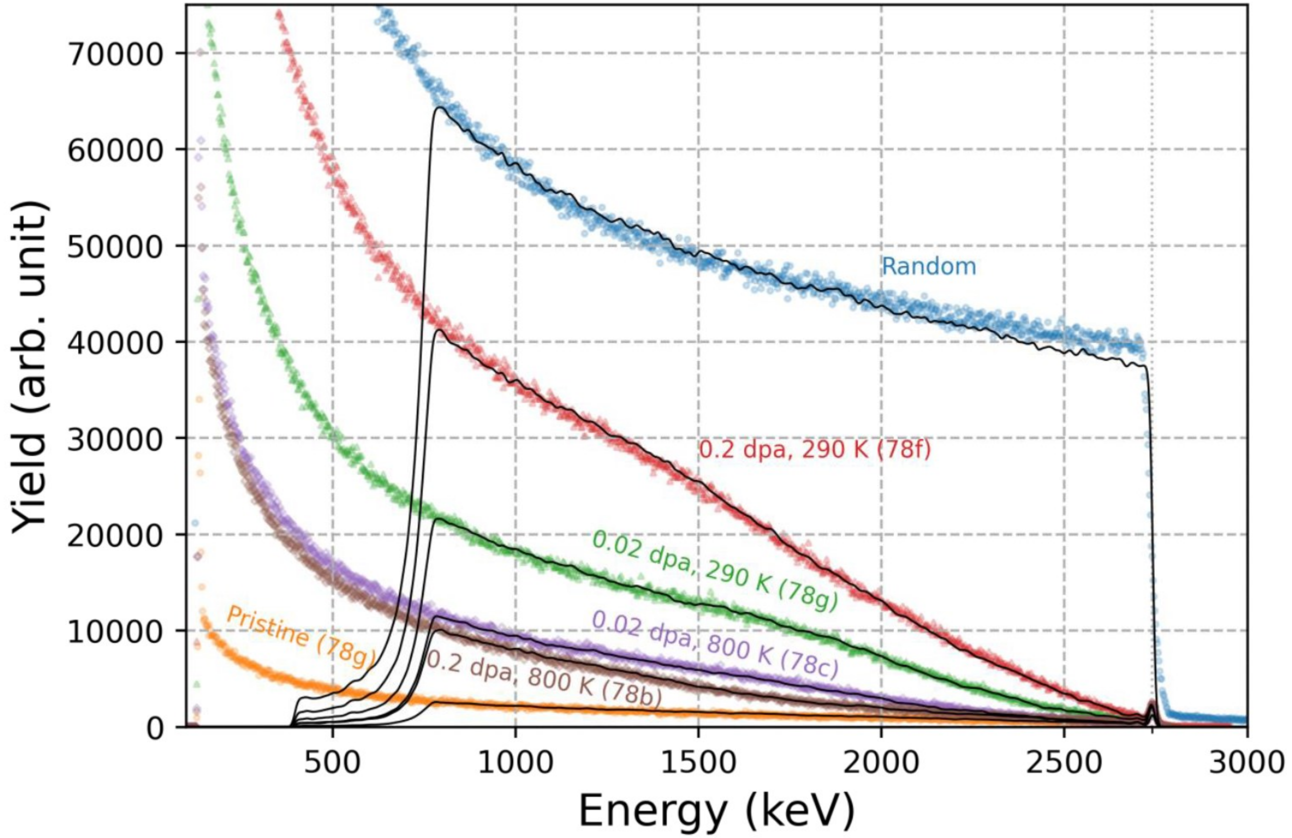
10.8 MeV W on W

Sample	Maximum dpa	Irradiation temperature (K)	Expectation of defects (DeHydroC meeting 07/10/2021)
78g	0.02	290	Single vacancies
78f	0.20	290	Heavily damaged
78c	0.02	800	Small vacancy clusters
78b	0.20	800	Big vacancy clusters



- **RBSADEC-Simulation:**
  - 2.987 MeV He ions on <111>-W
  - Detector: 170°
  - Temperature: 290 K
  - Detector resolution: 16.5 keV (FWHM)
  - Depth: 1.5 μm

- Random: a sample with 100 % randomly displaced atoms (RDA)
- Aligned-pristine: a perfect pristine sample (relatively high ion beam divergence)
- Aligned-damaged: samples with RDAs

Analysis of C-RBS spectra by RBSADEC simulation using randomly displaced atoms (RDA)

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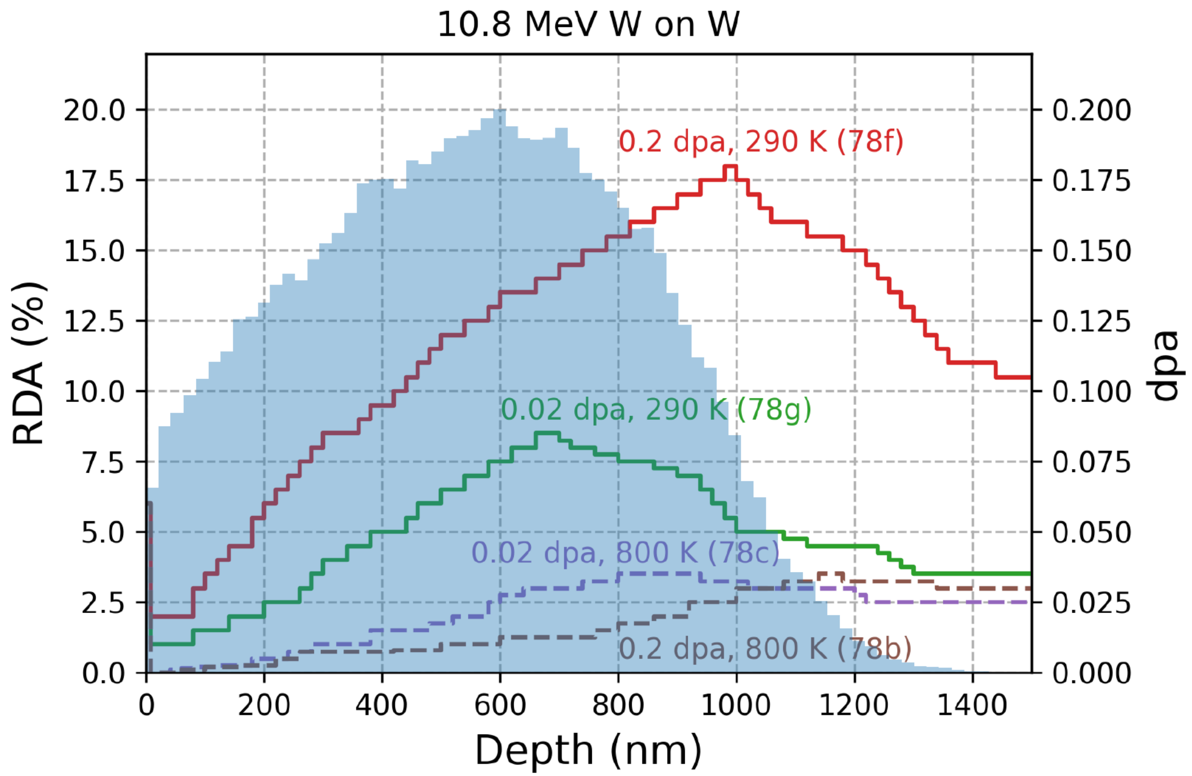
dpa profile

- SRIM - Full damage cascades
- 7° inclined
- Threshold displacement energy: 90 eV
- Maximum dpa: 0.2 at 600 nm



RDA profiles

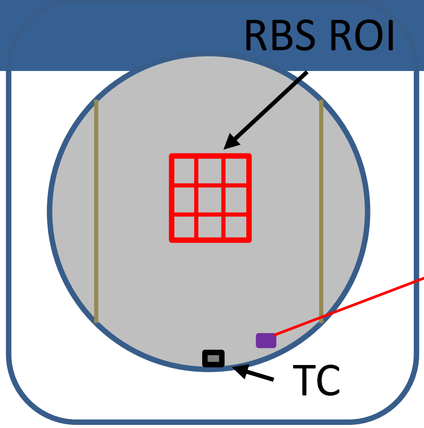
1) Surface disorder: 6 RDA in first 8 nm

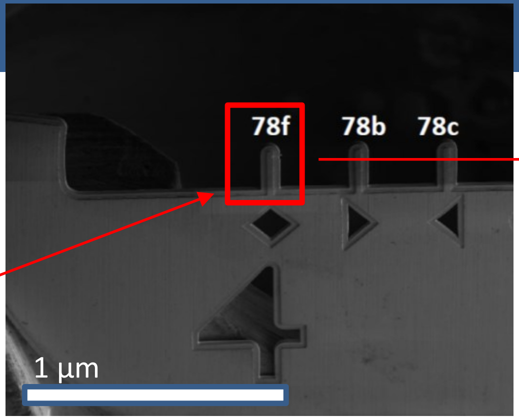
2) Maximum RDAs in bulk and corresponding depth

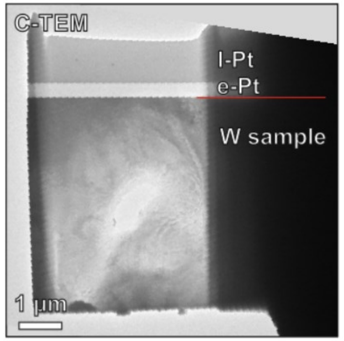
Samples	Max. RDA (%)		Depth (nm)	
78g (0.02 dpa, 290 K)	8.5	(not 10 times)	680	(higher)
78f (0.20 dpa, 290 K)	18		990	
78c (0.02 dpa, 800 K)	3.5	(same)	870	(higher)
78b (0.20 dpa, 800 K)	3.5		1160	

- No information about defect type
- RDA goes deeper than SRIM – clear misinterpretation: see STEM and TEM results

TEM analysis of SC W (111) samples after C-RBS



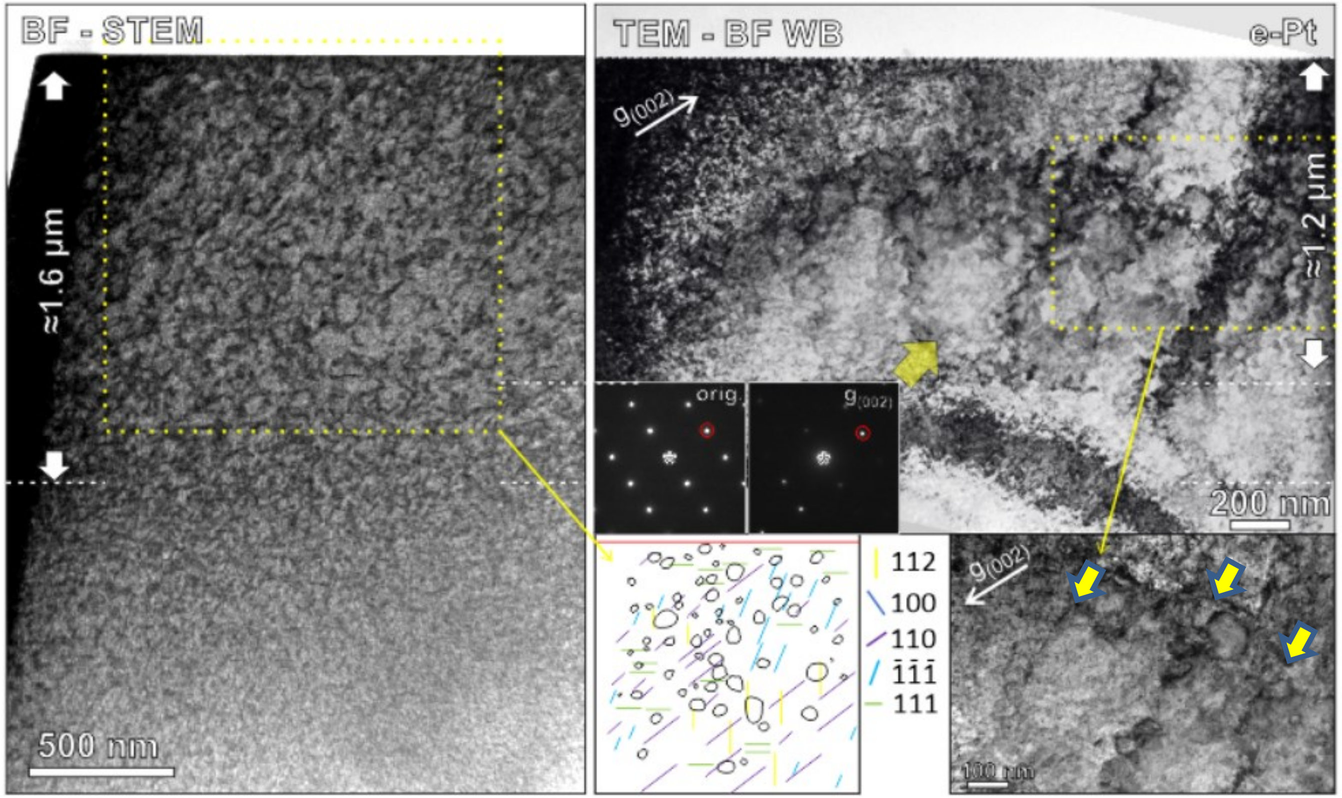




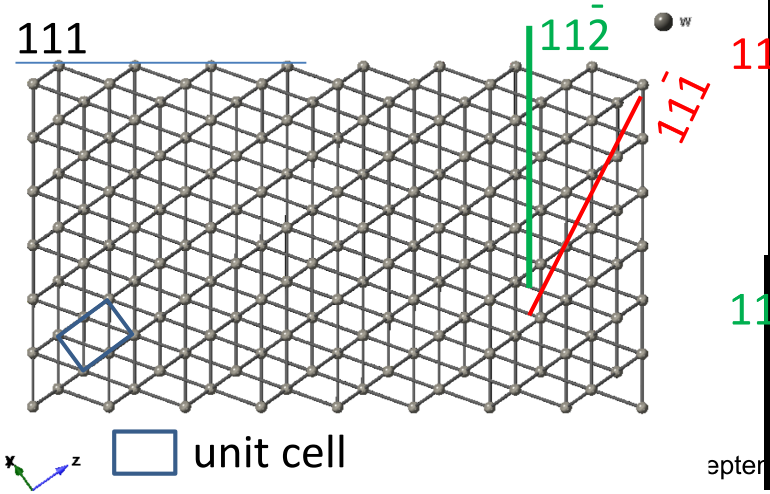
78f heavily damaged standard: 0.2 dpa 290 K

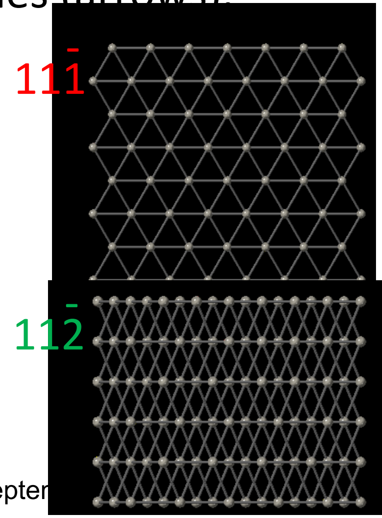
1. TEM sample prep by site-specific FIB

2. TEM lamella orientation and analysis (=> what we are looking at)



Bright-field (BF) STEM shows heavy defects in the first 1.6 µm below surface. Defects are mainly line dislocations following all major crystal planes, and dislocation loops (circles). As it appears, the DL loops are arranged / aligned along 11-1 planes (arrows).





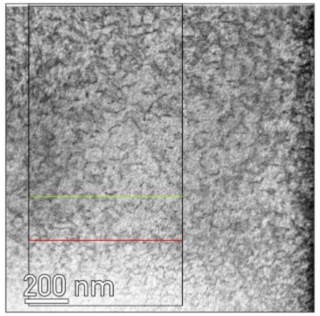
Jožef Stefan Institute

Summary page

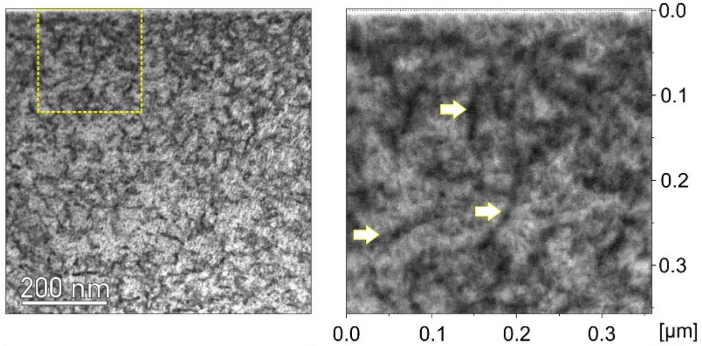
„DAMAGE“

„DEFECTS“

78f 0.2 dpa 290 K

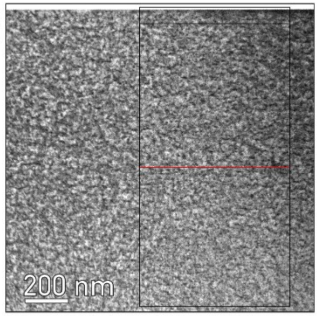
F


depth: (0.9-)1.1 µm

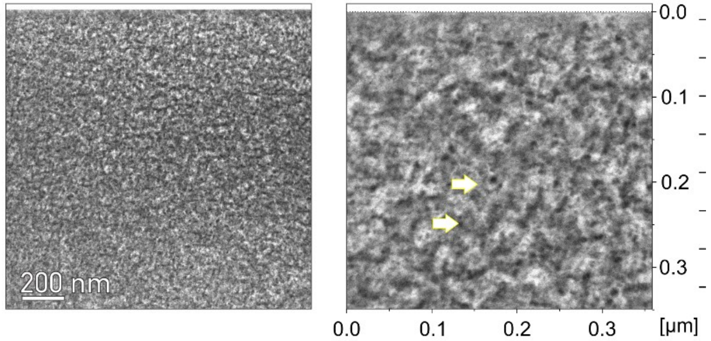
F


Dense network of dislocation lines (~100+ nm), which are already nicely visible at low-mag overview micrographs. Directions of DL lines coincide with 110 > 111 > 11-2 > 111 planes.

78g 0.02 dpa 290 K

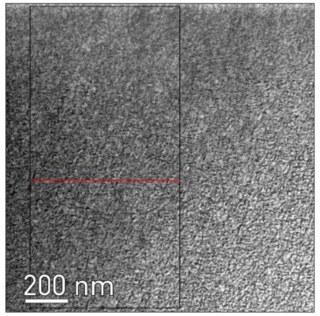
G


depth: 0.7 µm

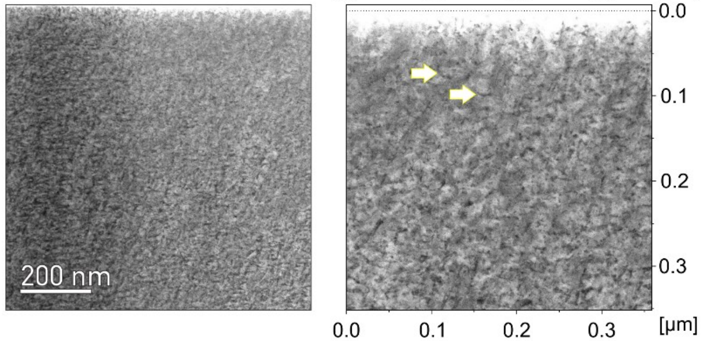
G


Only very short dislocation lines (~ 20-30 nm) in <111> , with prevailing U-shaped loops around “black dots” (size ~10 nm)

78c 0.02 dpa 800 K

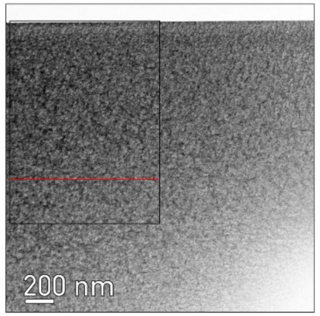
C


depth: 0.8 µm

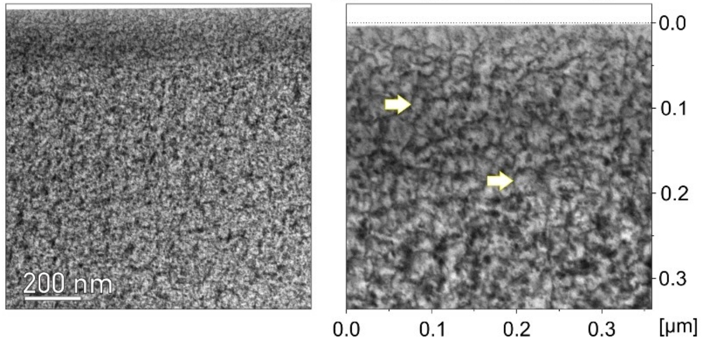
C


Dislocations: mainly dots and several isolated lines (< 50 nm, in <111> direction). Dots are smaller, several nm.

78b 0.2 dpa 800 K

B


depth: ~1.1 – 1.2 µm

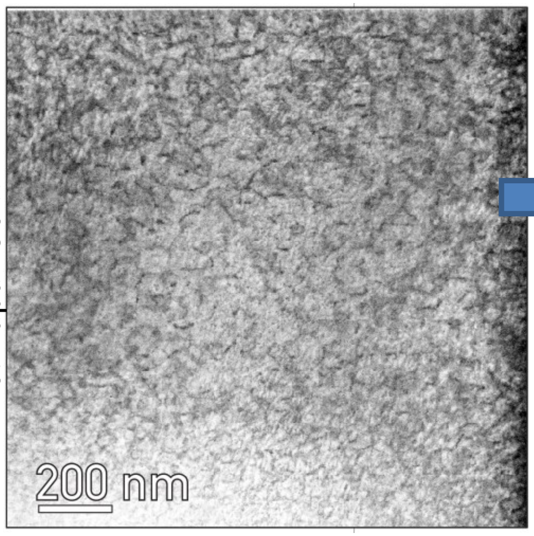
B


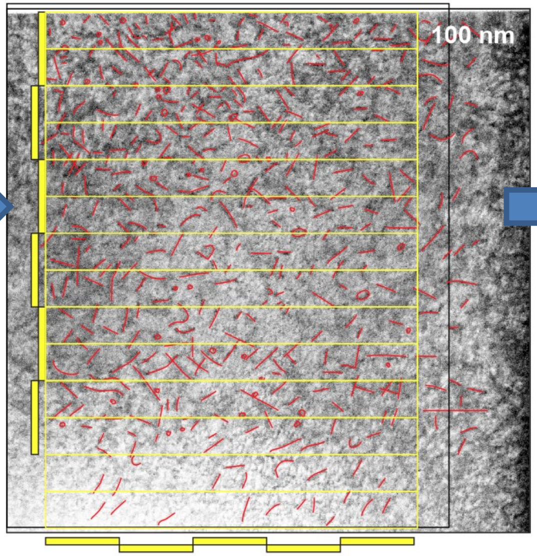
Several dislocation lines and larger black dots. DL lines are forming a network in <111>, forming square “polygons” with ~30 nm edge.

TEM analysis of SC W (111)

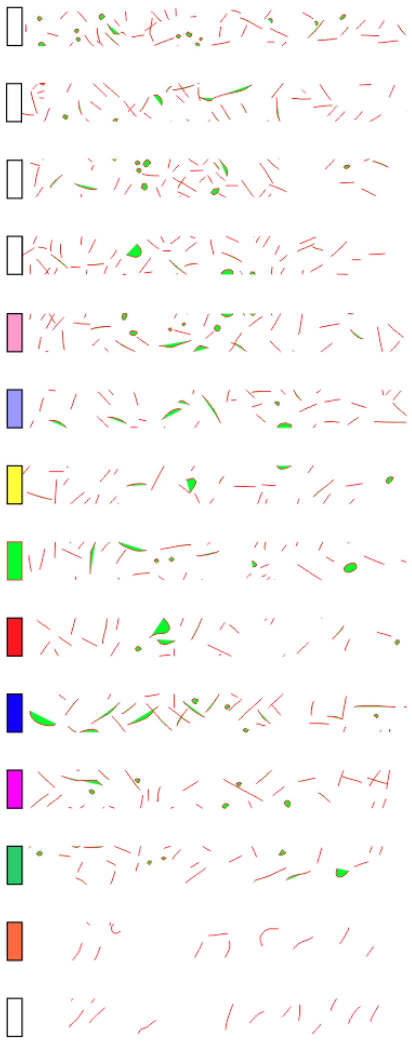
Average dislocation line density: 1.9 (±0.14) *E14 m/m³

0.2 dpa 290 K

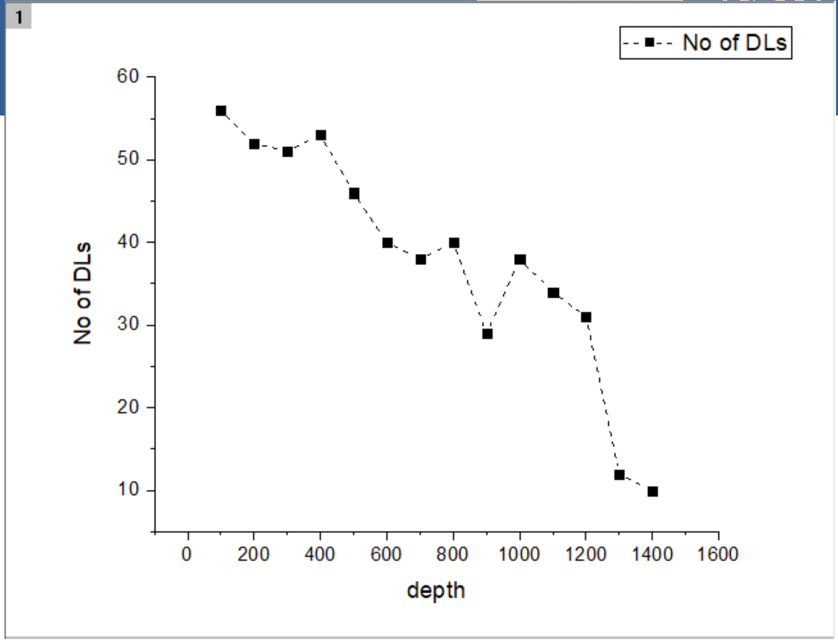


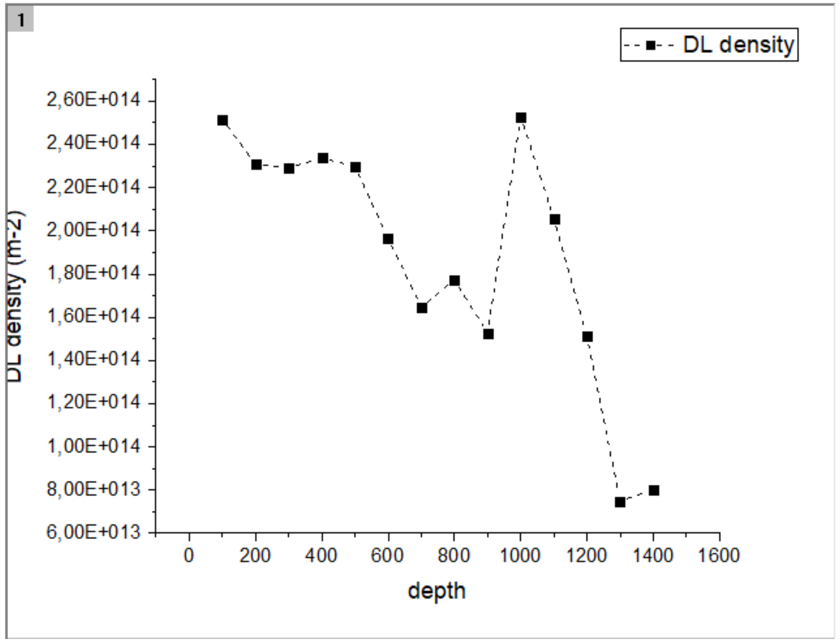


1000 nm



RANGE	No. of DLs	total length [nm]:		density
1. 000-100 nm	N = 56	length:	1760.8	2.52*E14
2. 100-200 nm	N = 52	length:	1615.9	2.31*E14
3. 200-300 nm	N = 51	length:	1604.0	2.29*E14
4. 300-400 nm	N = 53	length:	1636.1	2.34*E14
5. 400-500 nm	N = 46	length:	1608.0	2.30*E14
6. 500-600 nm	N = 40	length:	1376.0	1.97*E14
7. 600-700 nm	N = 38	length:	1152.7	1.65*E14
8. 700-800 nm	N = 40	length:	1240.8	1.77*E14
9. 800-900 nm	N = 29	length:	1069.3	1.53*E14
10. 900-1000 nm	N = 38	length:	1769.9	2.53*E14
11. 1000-1100 nm	N = 34	length:	1440.3	2.06*E14
12. 1100-1200 nm	N = 31	length:	1057.1	1.51*E14
13. 1200-1300 nm	N = 12	length:	524.4	7.49*E13
14. 1300-1400 nm	N = 10	length:	562.7	8.04*E13

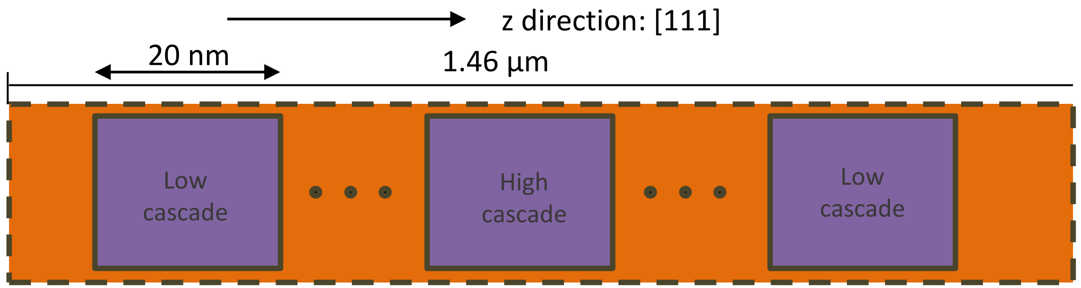


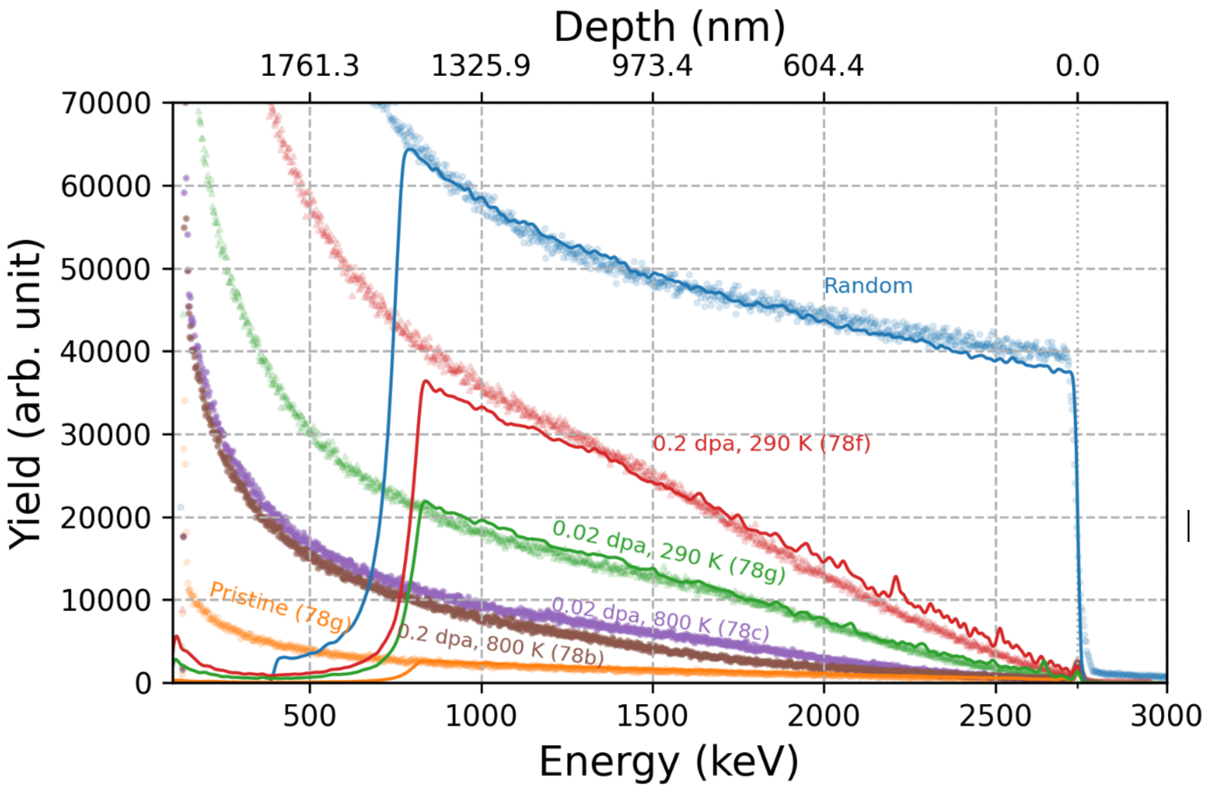


Calculations and fits of RBS/C spectra by RBSADEC simulation using MD cells

UNIVERSITY OF HELSINKI

- **Take real defect structures from MD**





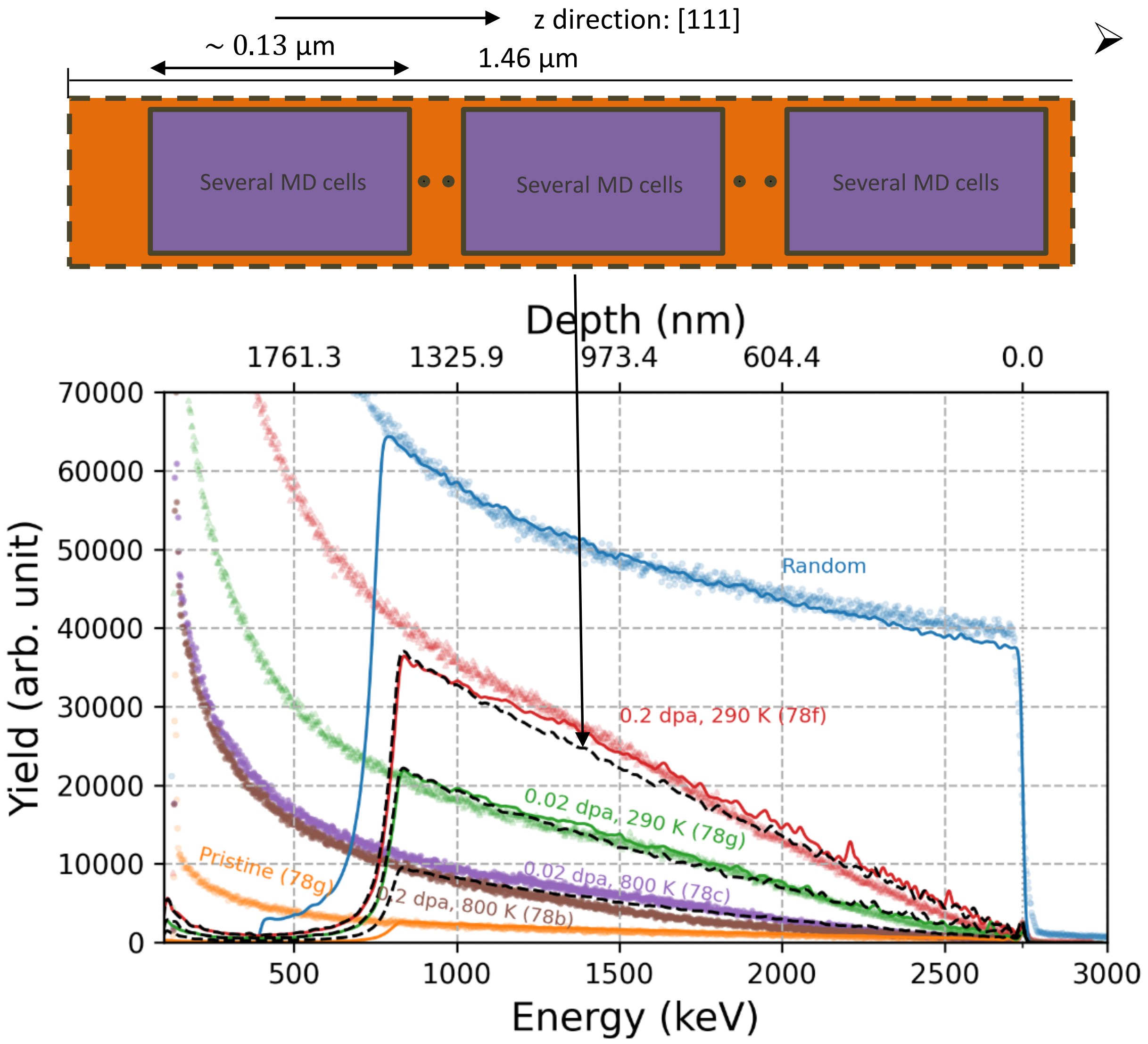
- **Generation of defects in MD cells**
  - **10 keV cascades**
  - **Collision cascade number ⟷ displacement damage dose**
- **Connection of W MD cells:**
  - The SRIM dpa depth profile is transformed to a collision cascade number profile.
  - Then MD boxes (70) with the corresponding cascade number are stacked along the direction of depth.

- Good agreement between simulation and experiment results (especially sample 78g)

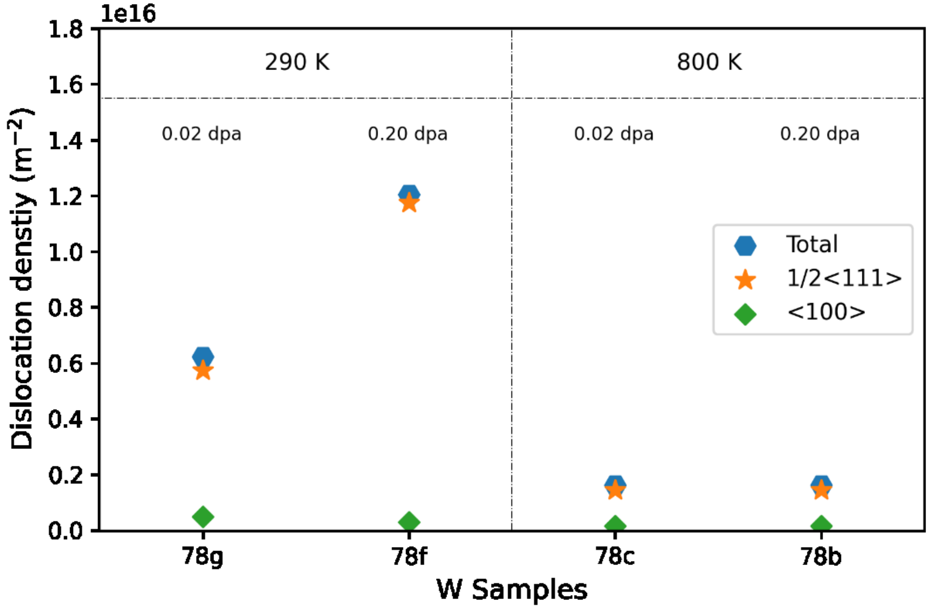
Calculations and fits of RBS/C spectra by RBSADEC simulation using MD cells

UNIVERSITY OF HELSINKI

- ❑ **Fits of RBS/C spectra by using several MD cells with certain cascade numbers – <u>part</u> of depth profile**



➢ **From this fitting method, we got the average dislocation density**



- ❑ **Comparison of simulation results from MD cells and RDA methods**
  - ➢ Damage range is overestimated by the RDA method (Low dechanneling induced by RDA)
- ❑ **Differences in dislocation density between simulation and TEM experimental results**
  - ➢ No dislocation line in MD cells - found by TEM **– work in progress**

Activities in first half of the project

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  - Task 4.1 Management.
  - Task 4.2 Dissemination, communication and exploitation

Development of NRA/C simulation and detection of D by RBSADEC code

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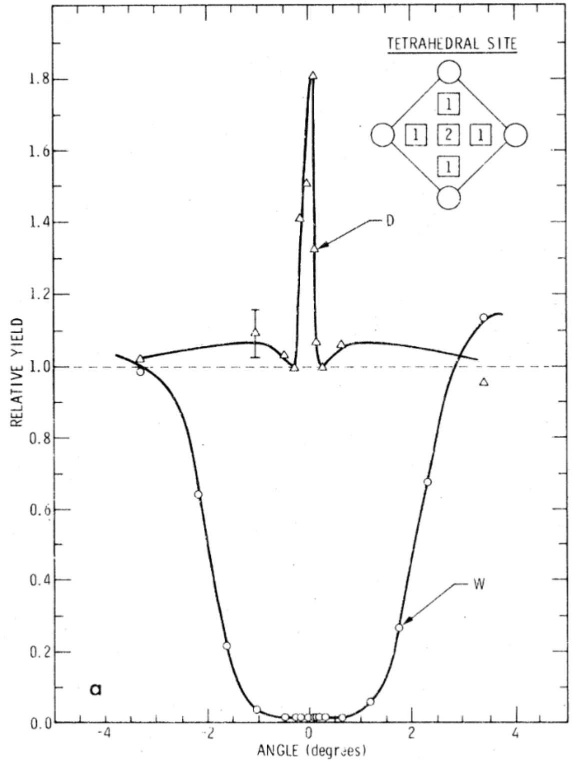
❑ Experiments in literature

- Incident ions: 750 keV ^3He ions
- Nuclear reaction: D (^3He, p) ^4He
- Detector angle: 135 degree
- Angular scan: around <100> axis of W
- D location: tetrahedral sites

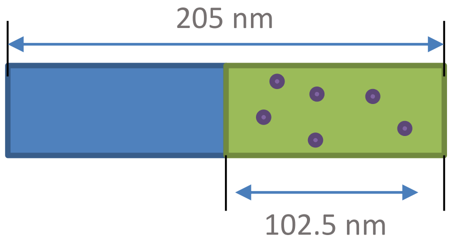


(S. Picraux, Phys. Rev. Lett., 33, 1974)

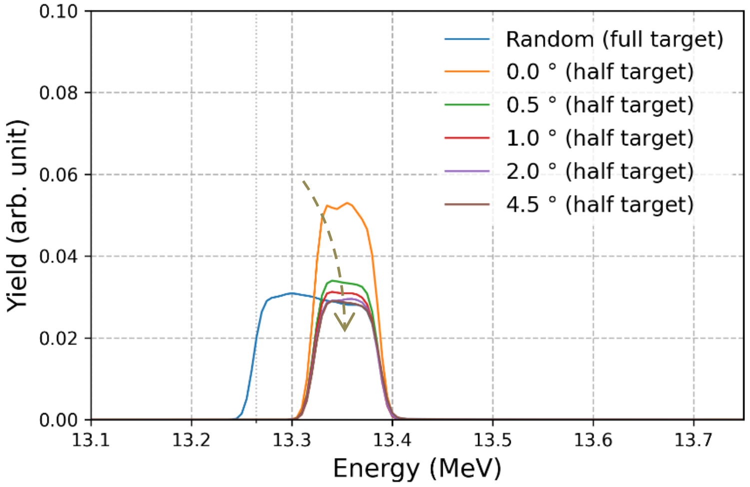
- Cross section data for D(^3He, p)^4He from Wielunska et al,NIM B, 371, 2014

❑ Example angular scans

- RBS/C: a pristine W target
- NRA/C:



- The first half is pristine: to establish a stable distribution of incident ions
- The second half : 0.1 % of D at tetrahedral sites



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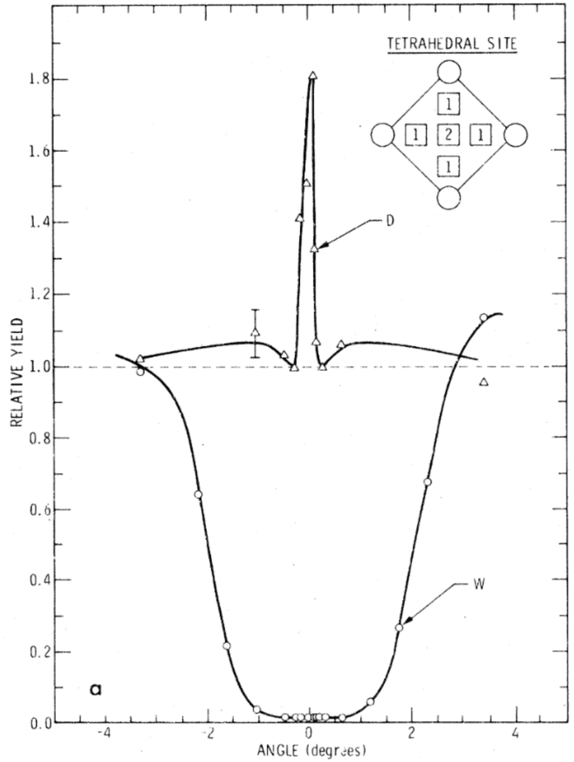
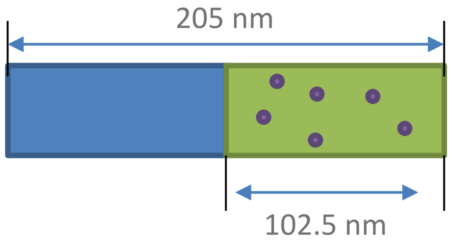


(S. Picraux, Phys. Rev. Lett., 33, 1974)

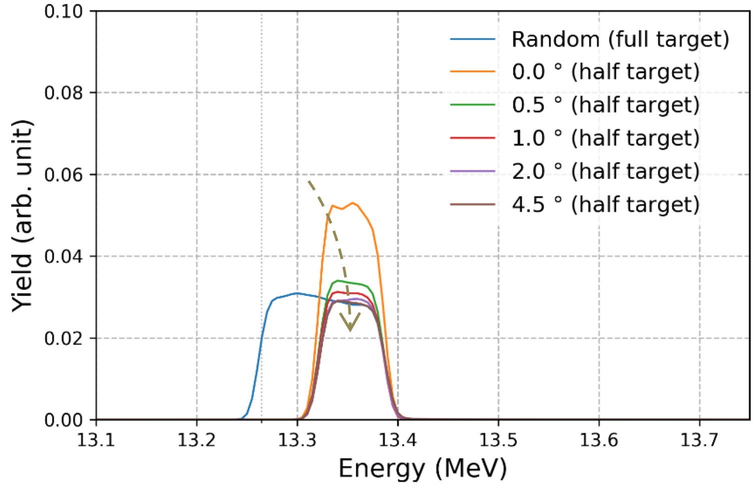
❑ Example angular scans

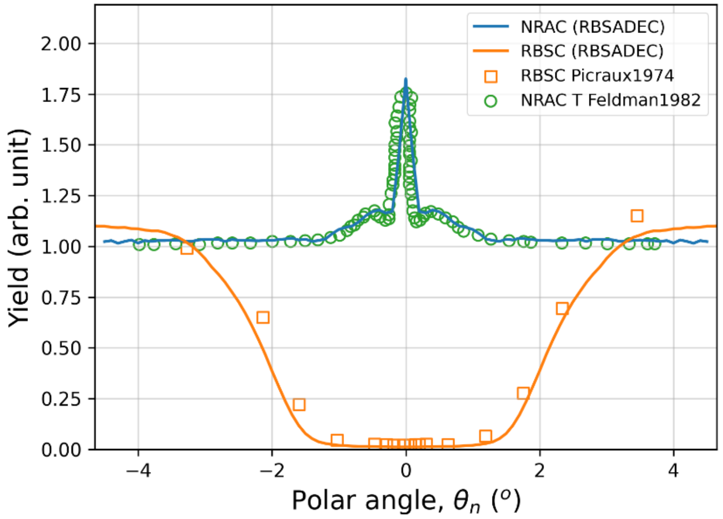
- RBS/C: a pristine W target
- NRA/C:



- The first half is pristine: to establish a stable distribution of incident ions
- The second half : 0.1 % of D at tetrahedral sites
- Comparison with NRA/C simulation in literature

(L. Feldman et al, Materials Analysis by Ion Channeling, 1982)





Development of NRA/C simulation and detection of D by RBSADEC code

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- Experiments in literature

- Incident ions: 750 keV ^{3}He ions
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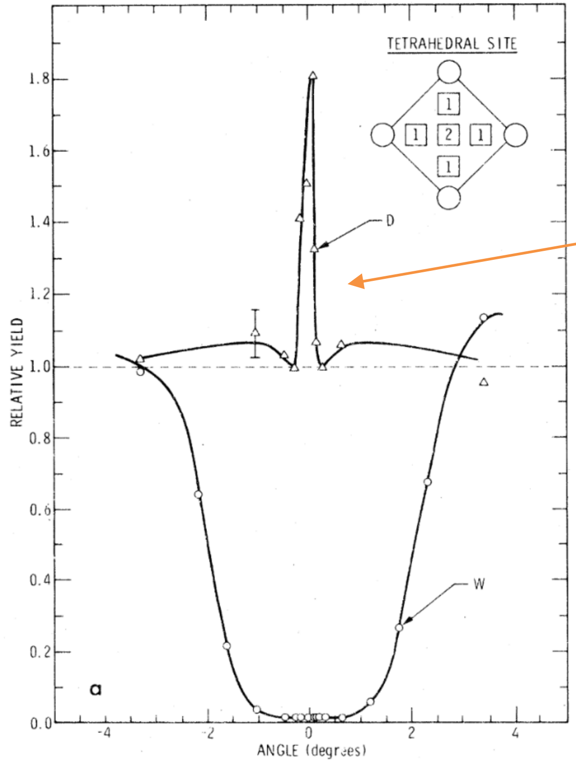
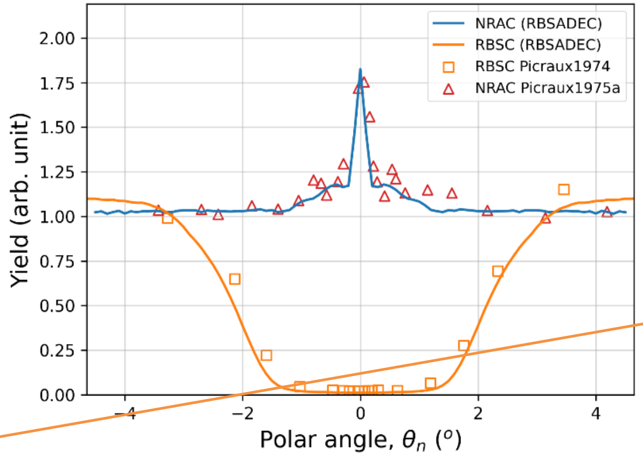
- Detector angle: 135 degree
- Angular scan: around <100> axis of W
- D location: tetrahedral sites



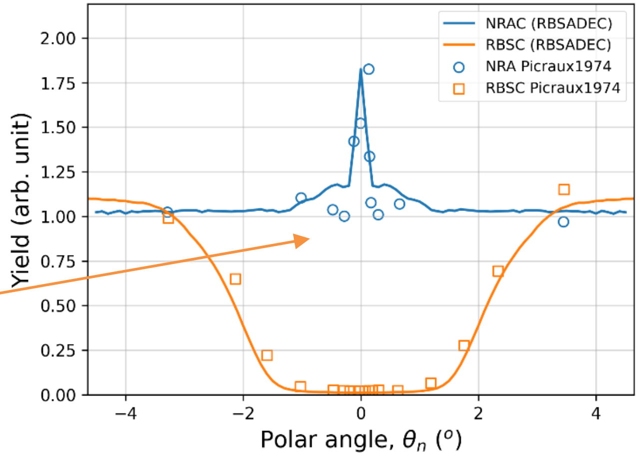
(S. Picraux, Phys. Rev. Lett., 33, 1974)

- Comparison between experiments and simulations



1×10^{15} cm^{-2} 15 keV D on W

(S. Picraux, Ion Implantation in Semiconductors, 1975, 355-360)



3×10^{15} cm^{-2} 30 keV D on W

(S. Picraux, Phys. Rev. Lett., 33, 1974)

- Small difference between experiments and simulations: not exactly on tetrahedral sites? – Vacancies, some position close to tetrahedral sites, etc.
- Effect of damage dose: D sites change

➢ **Future: Improving the fit: adjust D locations**

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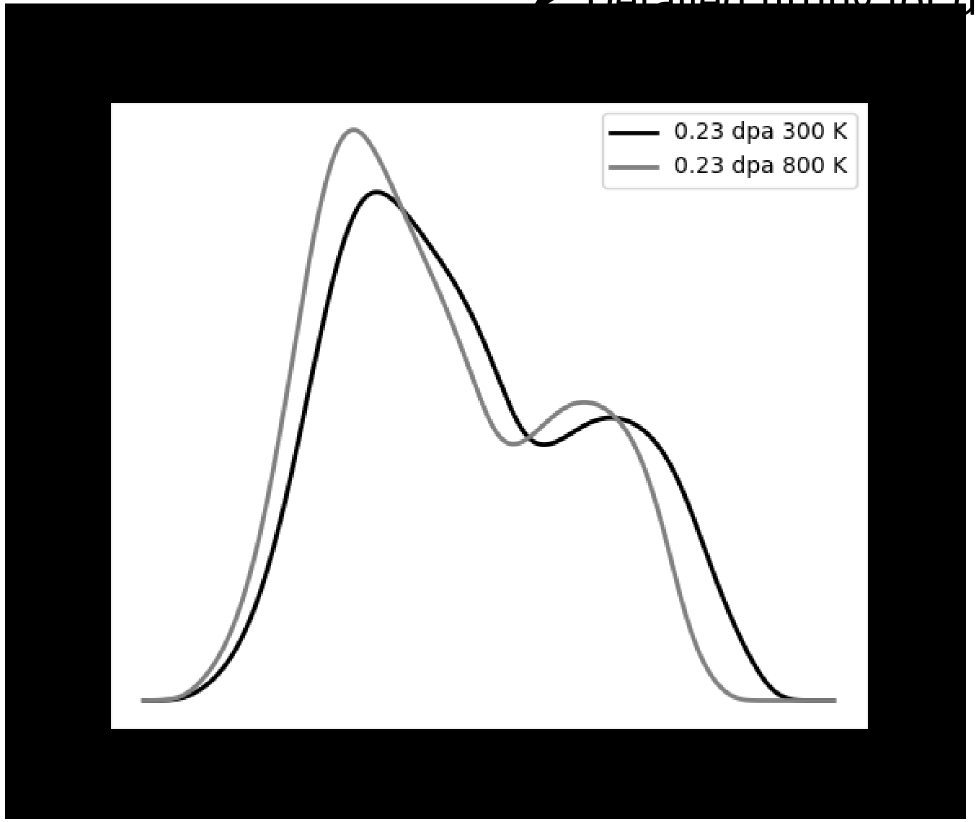
Macroscopic Rate Equation (MRE) modelling with MHIMS code: Simulated TDS spectra

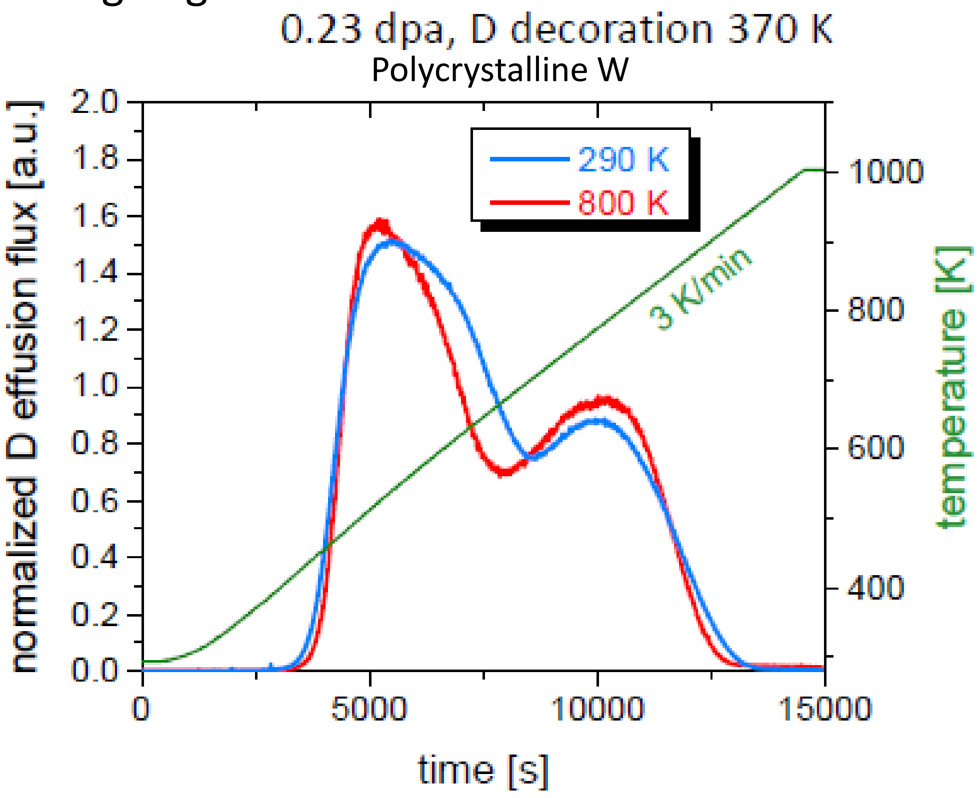
- **From fitting the D depth profiles and TDS spectra we obtain the information of defect concentration and de-trapping energies for different damaging scenarios**
- Input for RBSADEC code / Compare to MD simulations

Comparison of simulated and experimental TDS spectra between damaging at 300 K and damaging at 800 K

- Detailed fitting for different dpa ongoing

$$\frac{\varphi_{\mathrm{des}}(t)}{\int \varphi_{\mathrm{des}}(t)dt}$$





Management

- **WP 4 management -** seven zoom meetings organized with the team members, details and presentations available on Indico, links to indico sites on Wiki page https://wiki.euro-fusion.org/wiki/Project_No4
- Kick off Meeting – April 2021
- Status meeting in June 2021
- October 2021
- November 2021
- February 2022
- June 2022
- September 2022

Status of the project and future plans

Project is proceeding as planned

On schedule
Delayed
To be started

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Thank you for your attention