Displacement damage stabilization by hydrogen presence under simultaneous W ion damaging and D ion exposure

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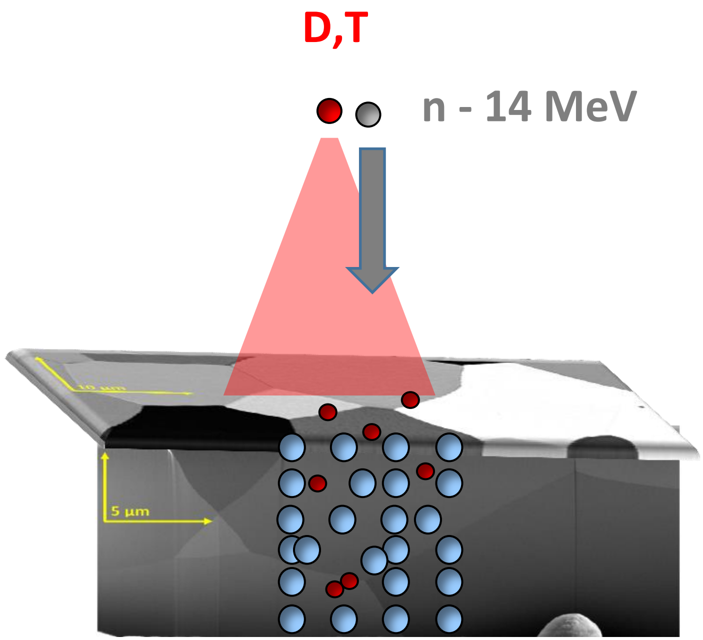
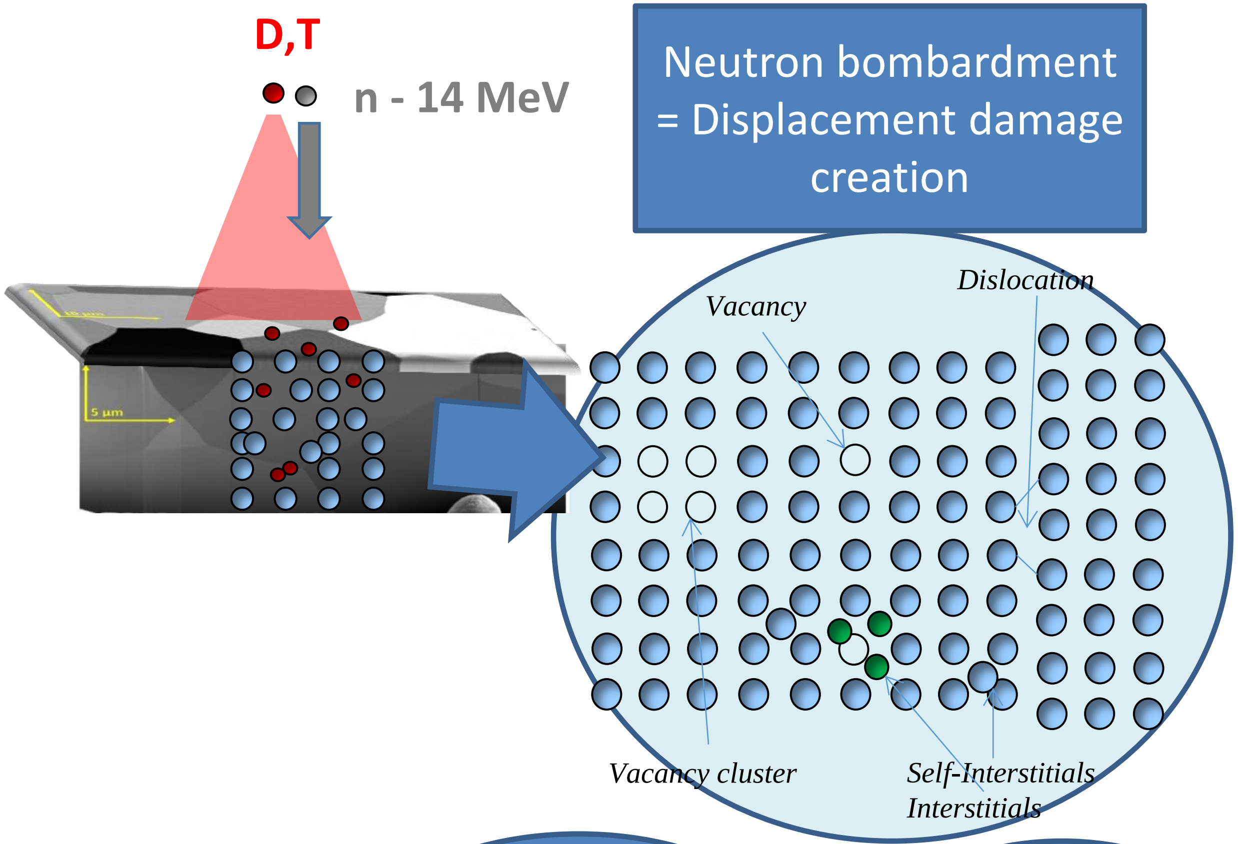
Tungsten –plasma facing material

Fusion device scenario

D/T plasma exposure + neutron irradiation



Tungsten –plasma facing material



Neutron bombardment = Displacement damage creation

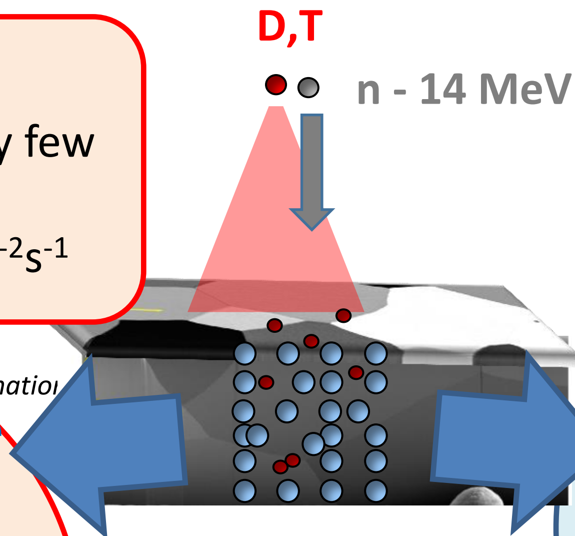
Damage creation at RT + damage annealing

Damage creation at elevated temperatures

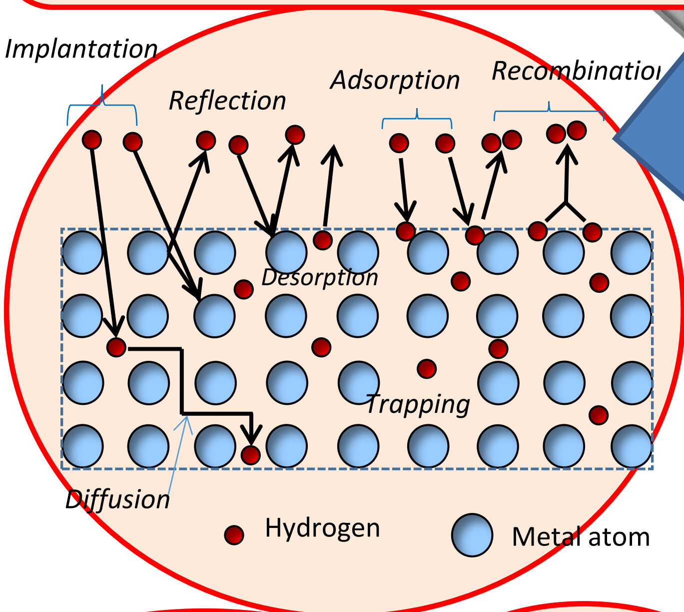
Tungsten –plasma facing material

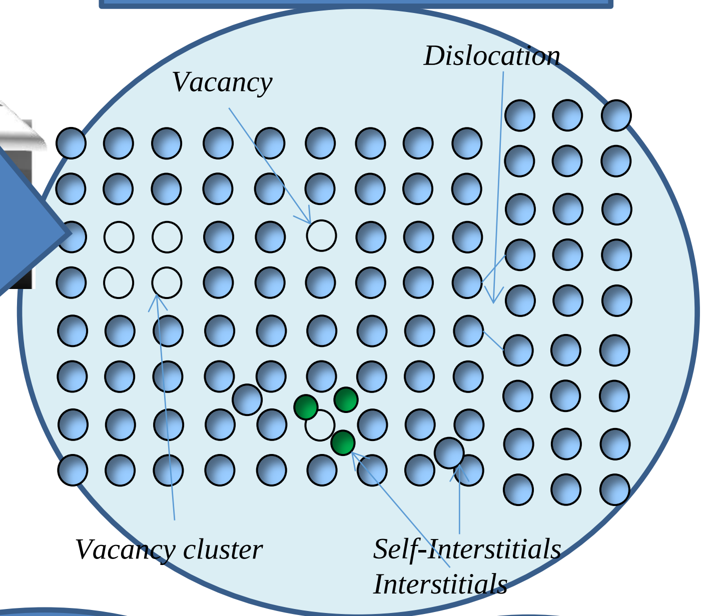
Fuel implantation

- ions and neutrals - energy few eV – keV;
- High fluxes up to $10^{24}\ m^{-2}s^{-1}$



Neutron bombardment = Displacement damage creation





Fuel transport: diffusion trapping de-trapping

Fuel retention

Damage creation at RT + damage annealing

Damage creation at elevated temperatures

Tungsten –plasma facing material

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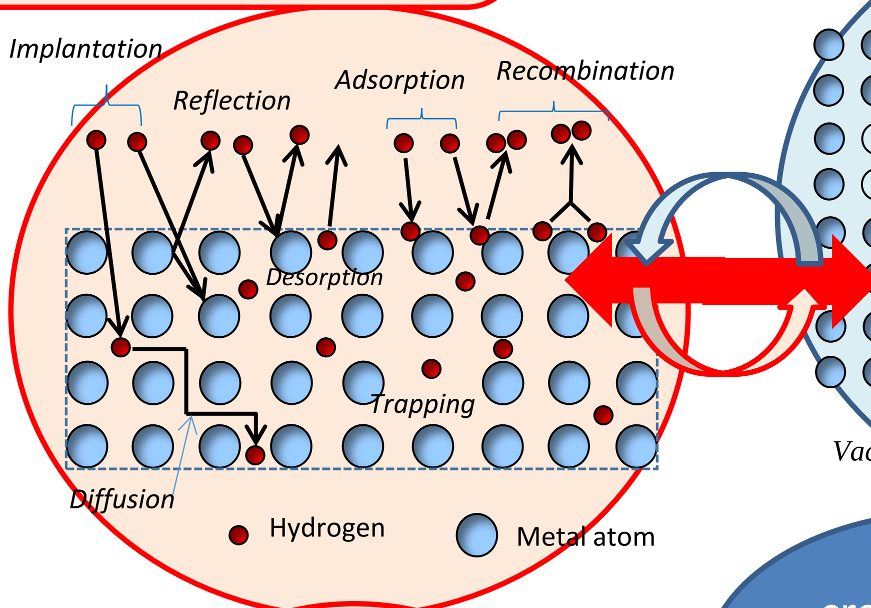
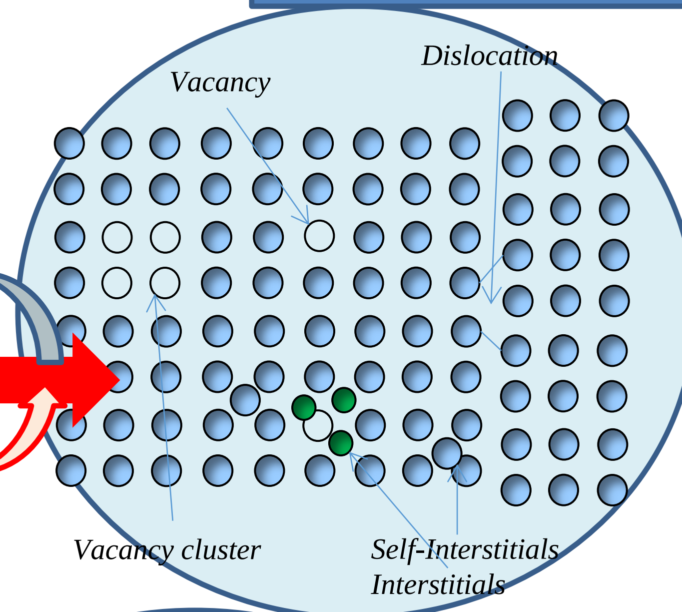
Fuel implantation
- ions and neutrals - energy few eV – keV;
- High fluxes up to 10^{24} $m^{-2}s^{-1}$

Neutron bombardment = Displacement damage creation





Fuel transport:
diffusion
trapping
de-trapping

Fuel retention

Damage creation at RT
+
damage annealing

Damage creation at elevated temperatures

Outline

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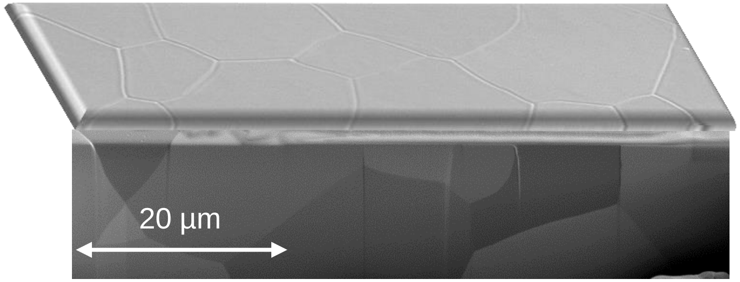
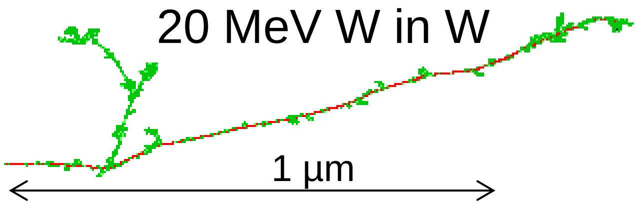
- *Different displacement damaging procedures*
- *Comparison between:*
  - *Sequential W ion irradiation and D exposure*
  - Simultaneous *W ion irradiation and D exposure*
- *Comparison atoms versus ions*
- Conclusions

14 MeV neutron irradiation
Displacement damage creation



W self-damaging



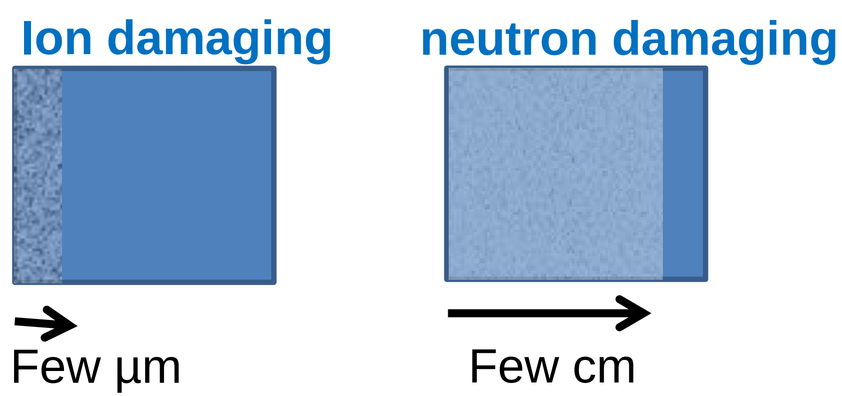
SRIM calculation of ion trajectory

Influence of neutron irradiation on D retention
activation of samples, long irradiation time,
14 MeV neutrons not available (fission neutrons)!

High energy ion damaging

MeV W ion irradiation = Surrogate for neutron irradiation

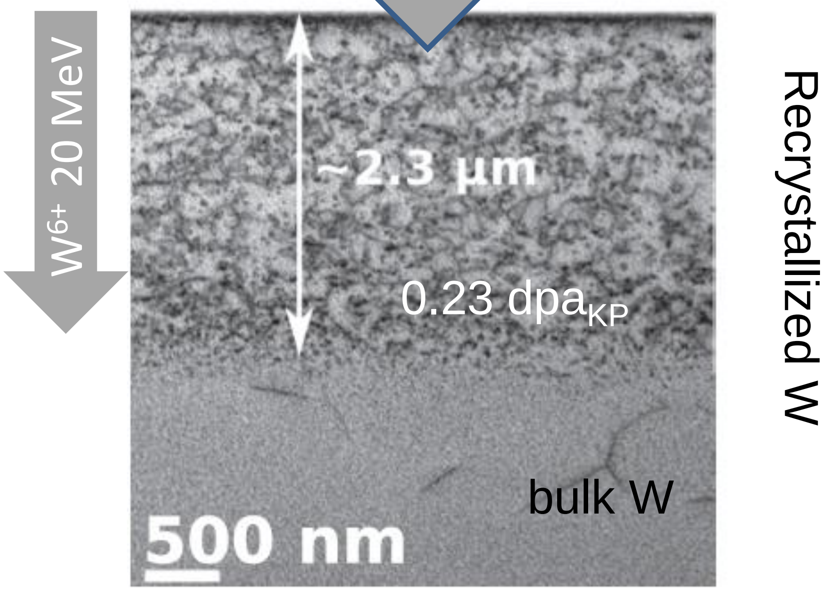
- Dense cascades and no chemical effect
- No transmutation



Displacement damage creation
MeV W ion irradiation

W self-damaging

W ions 20 MeV | 7.9×10^{17} W/m^2



Damaged layer characterization by Scanning Transmission Electron Microscopy [Zaloznik et al. Phys Scr. T167 (2016) 014031]

<u>W ion irradiation by MeV W ions</u>

- Creation of displacement damage

Displacement damage creation
MeV W ion irradiation

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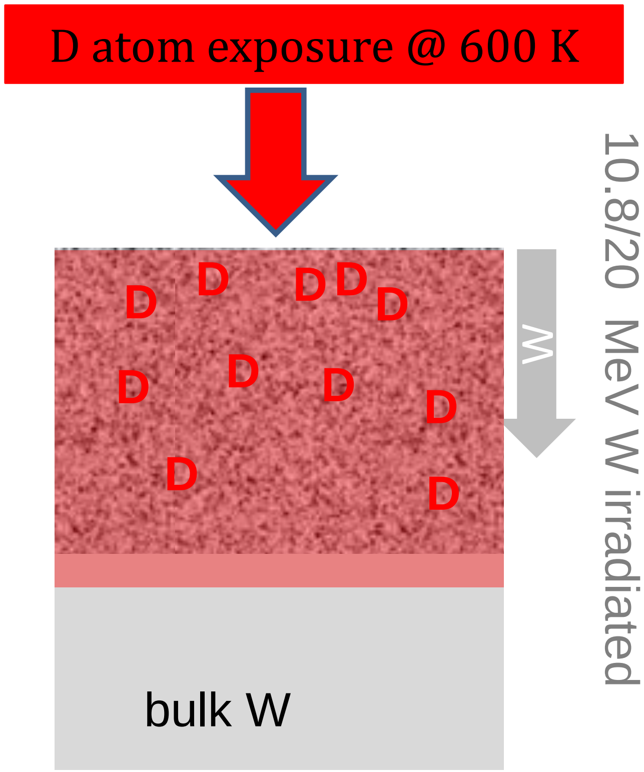
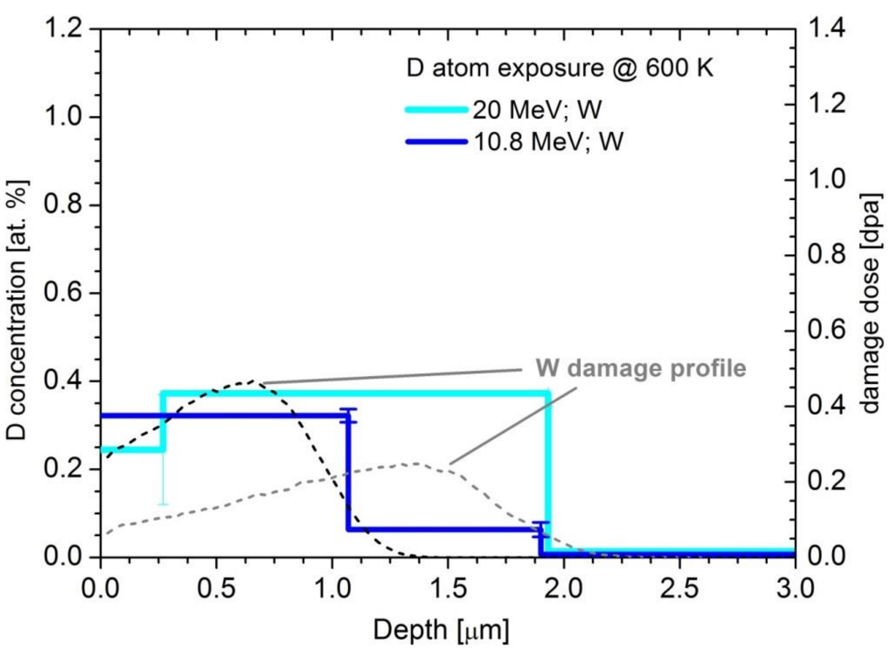
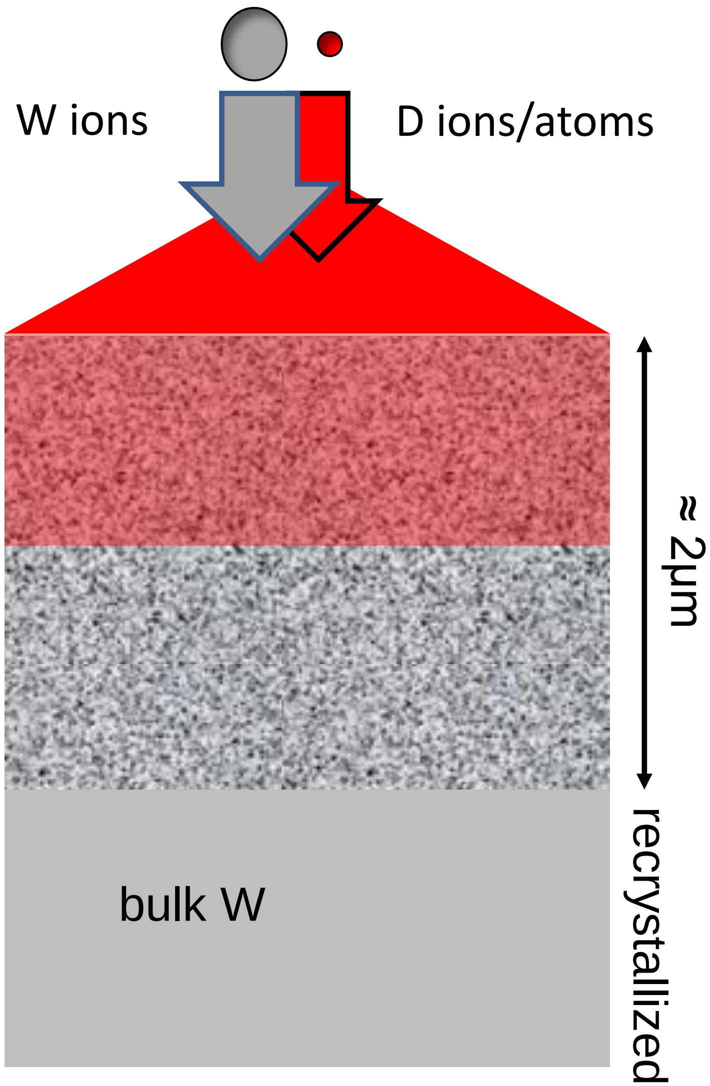
W ion irradiation by MeV W ions

- Creation of displacement damage
- Increased fuel retention in ion damaged W material from ~ 10^{-3} at. % ↗ ~ 1 at. %
- D saturation observed at damage dose > 0.2dpa for RT W irradiation! [Alimov et al. JNM 2013, Hoen et al. NF 2012, Schwarz-Selinger FEC 2018]





Simultaneous W/D exposure

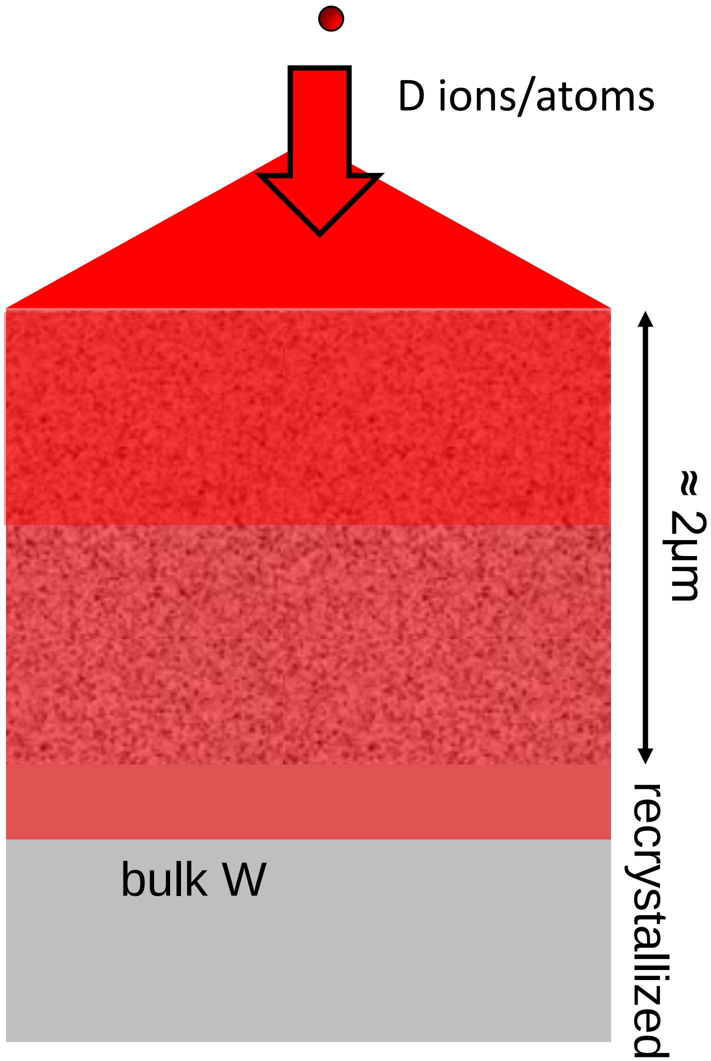


Simultaneous W/D exposure:

W ion irradiation
D exposure

@ different high temperatures

Simultaneous W/D-D exposure



Simultaneous W/D-D exposure:

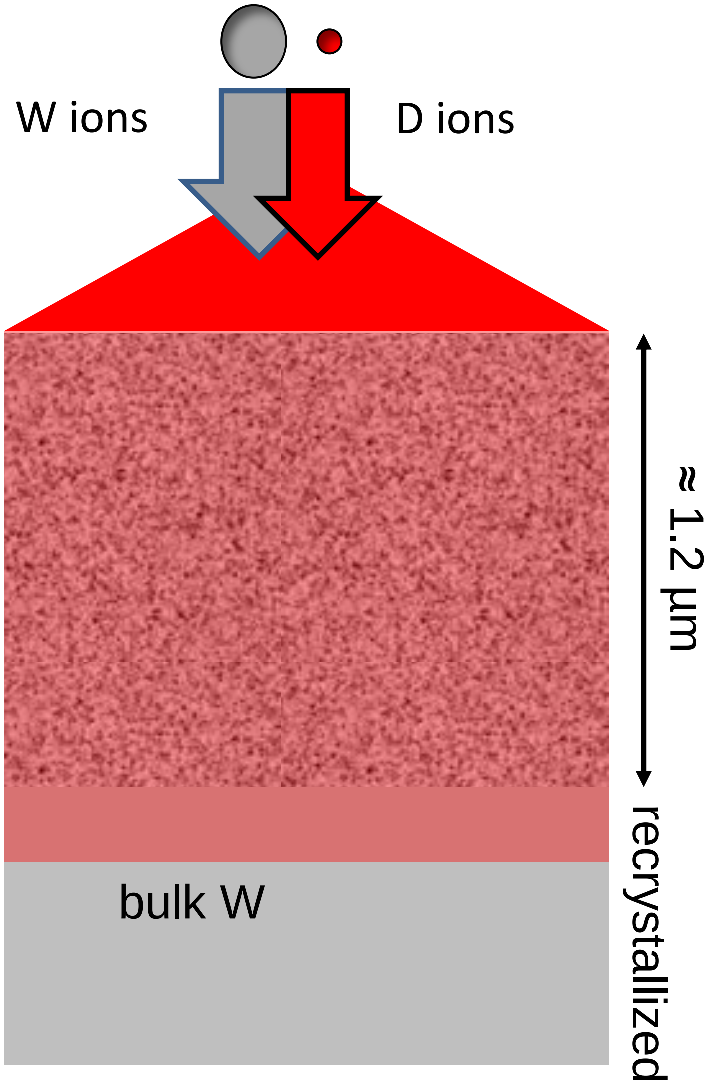
W ion irradiation **@ different high temperatures**
D exposure

-

D exposure **@ low temperature to populate created traps**

✓ D retention a way to determine defect concentration

Sequential W-D exposure



Sequential W-D exposure:

W ion irradiation @ different high temperatures

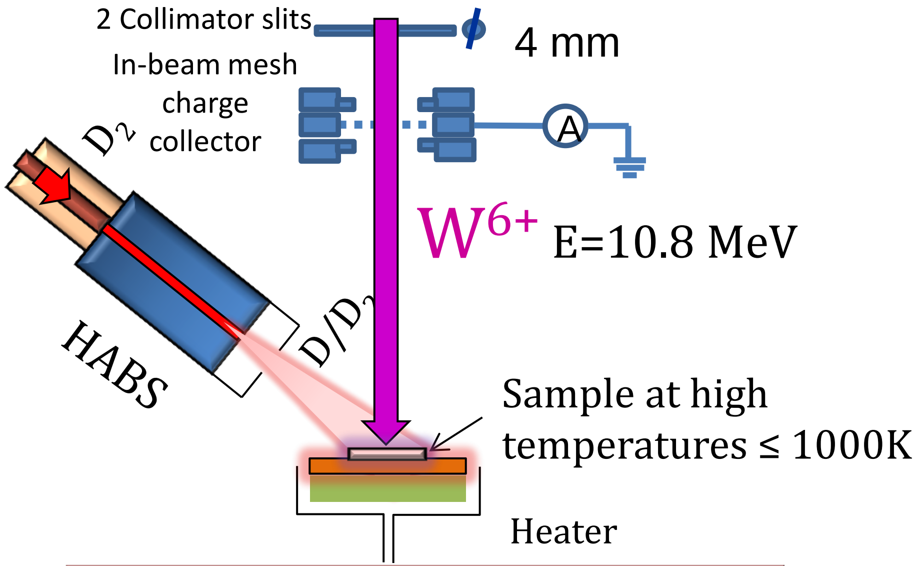
-

D exposure @ low temperature to populate created traps

✓ D retention a way to determine defect concentration

Experiment with atoms – 0.28 eV/D

- Simultaneous/sequential W/D, W-D atom loading
- Defect population - exposure D atoms @ 600 K – fluence 3.7 ×10^{23} D/m^2



Simultaneous/sequential W irradiation and D atom exposure at high temperatures for 4 h

Atom flux=5.4x10^{18} D/m^{2}s
Γ_D=8x10^{22} D/m^2

W fluence = 1.4x10^{18} W/m^2
Dose→ 0.47 dpa$_{KP}$
Displ. Rate = 3*10^{-5} dpa/s

Analysis methods:

- Deuterium depth profile measurement by Nuclear Reaction Analysis (NRA)
- TDS – final step – D desorption kinetics and D amount

Effect of D presence – atom exposure
Comparison of D concentration

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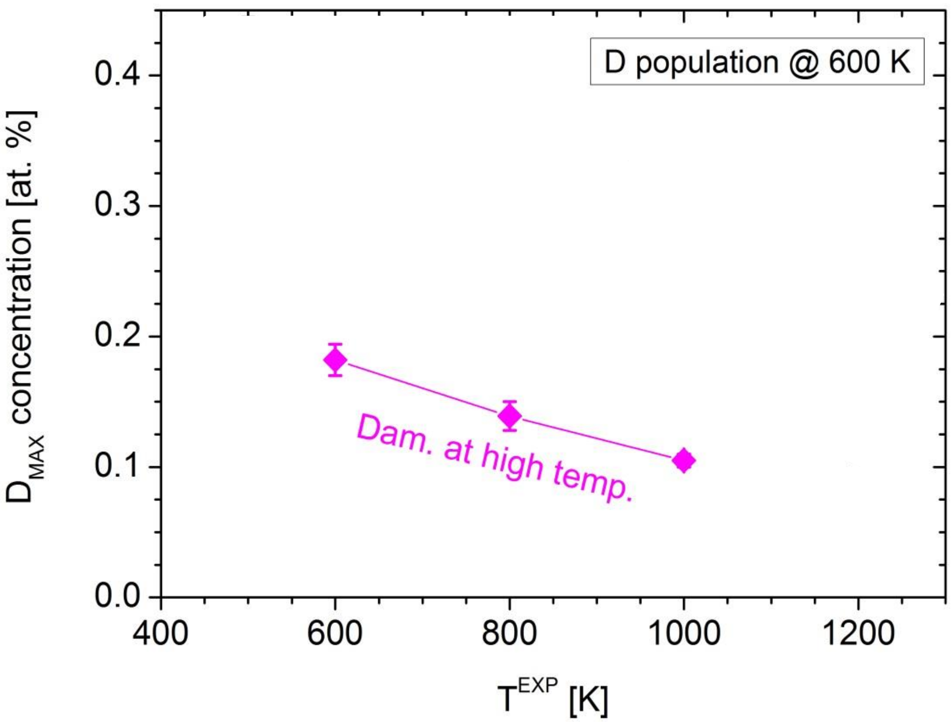
- Neutron damaging simulated by self implantation
- <u>Simultaneous W ion damaging and D atom loading</u>

<u>Comparison to different damaging procedures</u>

- *Sequential: Damage at T^{EXP}; D population at 600 K*



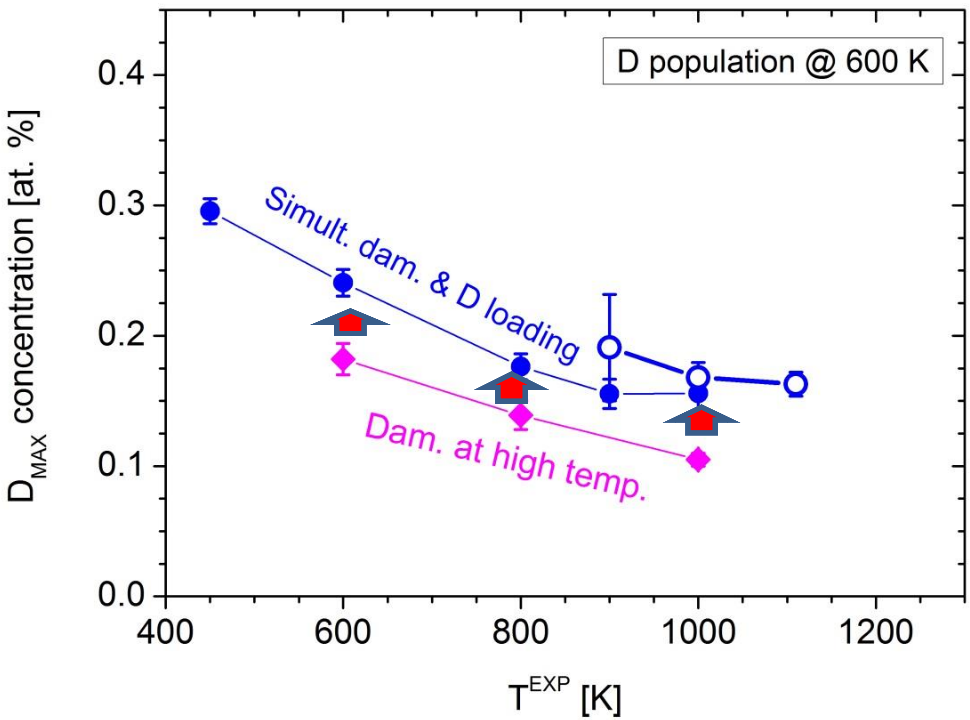
Effect of D presence – atom exposure
Comparison of D concentration

WP PFC

- Neutron damaging simulated by self implantation
- Simultaneous W ion damaging and D atom loading

Comparison to different damaging procedures

- *Sequential: Damage at T^{EXP}; D population at 600 K*
- *Simultaneous: Damage & D exposure at T^{EXP}; D population at 600 K*



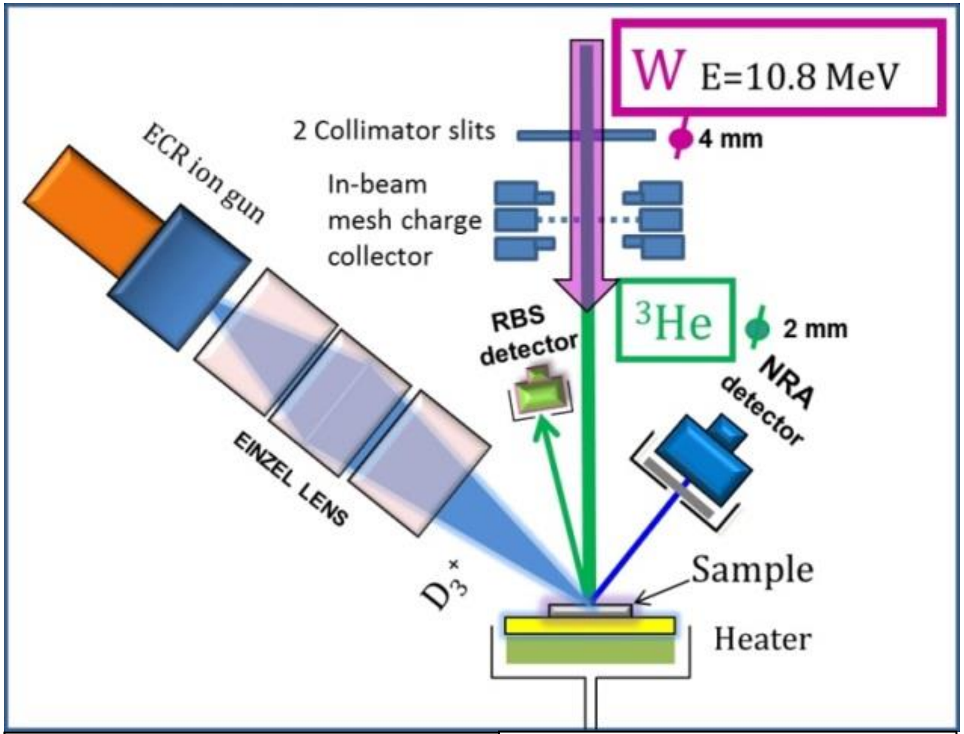
- ✓ ***Observed synergistic effects but not dramatic – 30 % increase***
- ✓ **Competition between defect annihilation at elevated temp. and defect stabilization by D**

For more details see:

- S. Markelj, et al, Nuclear Materials and Energy 12 (2017) 169.
- E. Hodille et al. Nucl. Fusion **59** (2019) 016011

Experiment with ions– 300 eV/D

- <u>Simultaneous/sequential W/D, W-D ion loading</u>
- <u>Defect population - exposure D ions @ 450 K – fluence 2.7×10^{23} D/m^{2}</u>



Ion energy 300 eV/D Ion flux=1.3x10^{18} D/m^{2}s Γ_D=1.9x10^{22} D/m^2	W fluence = 1.0x10^{18} W/m^2 Dose→ 0.35 dpa$_{KP}$ Displ. Rate = 2.4*10^{-5} dpa/s

Analysis methods:

- Deuterium depth profile measurement by Nuclear Reaction Analysis (NRA)
- TDS – final step – D desorption kinetics and D amount

- S. Markelj et al, Nucl. Fusion (2019) in press
- M. Pecovnik et al. submitted to Nucl. Fusion

TDS - Sequential experiment

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W ion damaging at 300 K – sequential

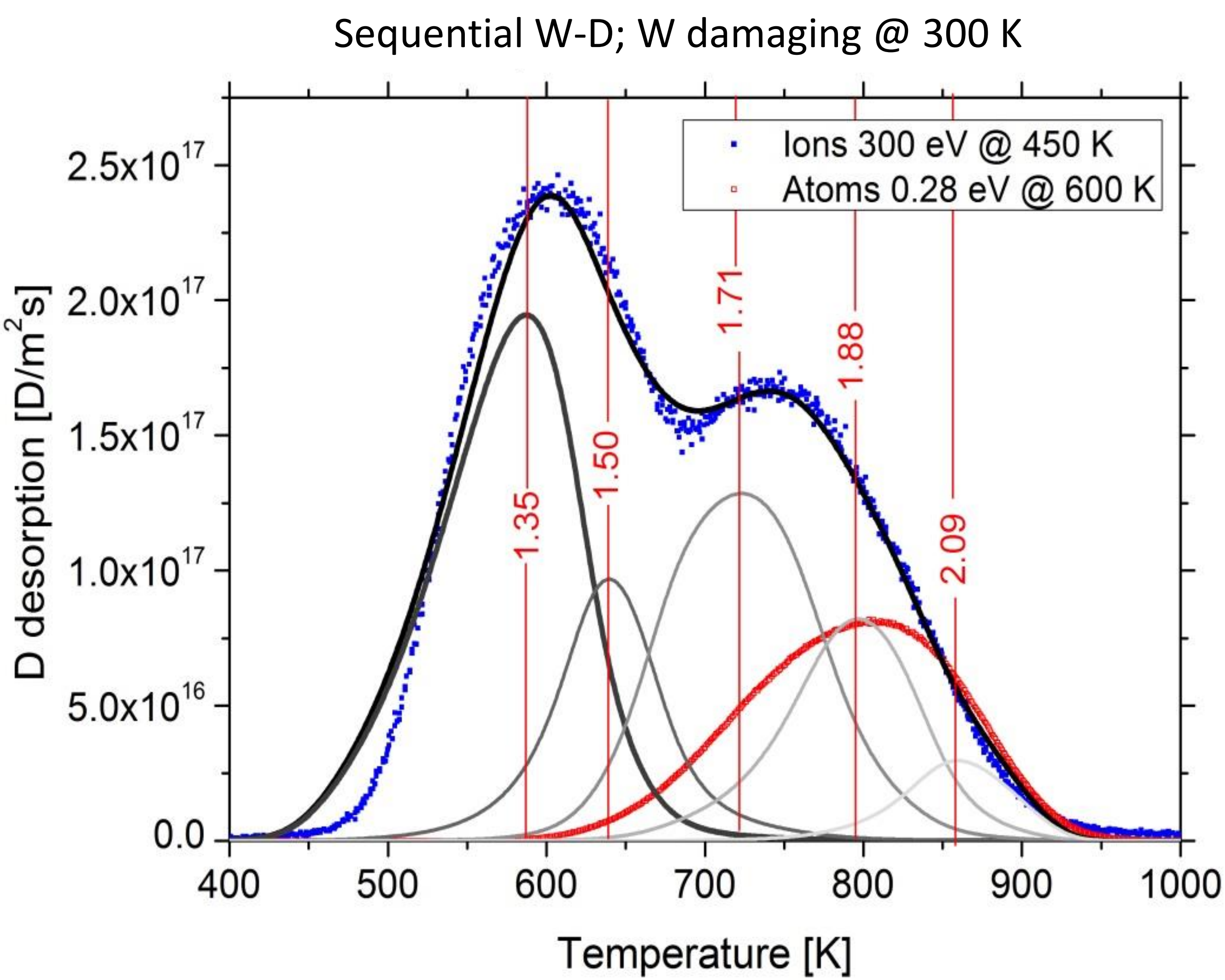
D atom exposure at 600K

- ✓ Single peak
- ✓ Two de-trapping energies 1.82 eV and 2.06 eV

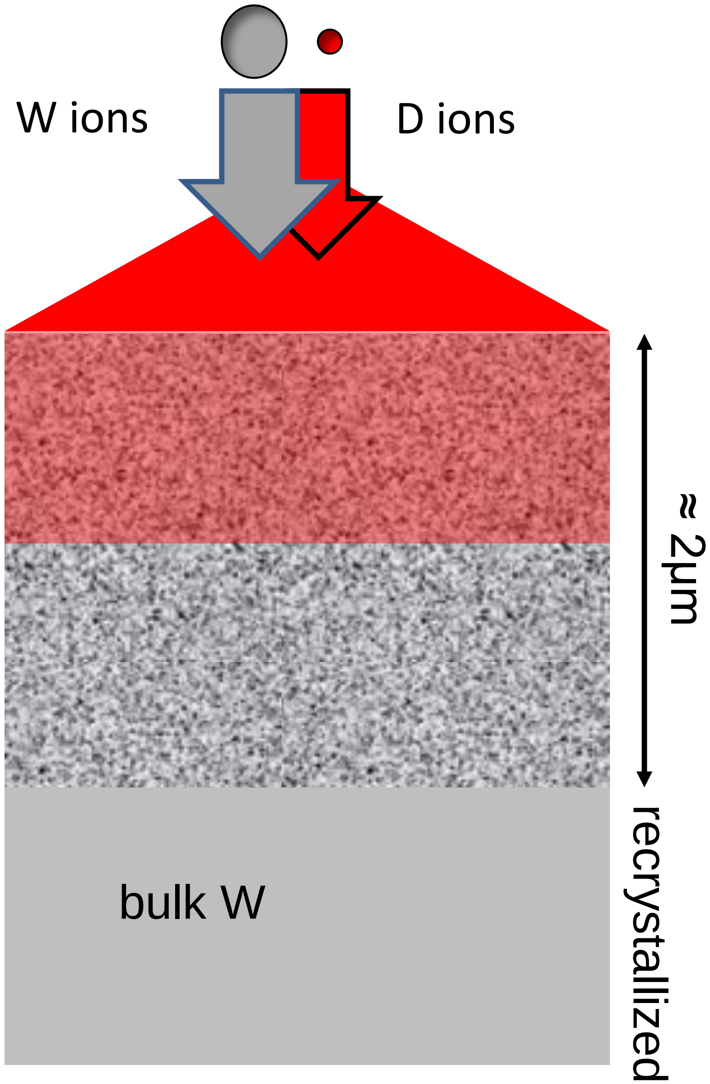
D ion exposure at 450K

- ✓ Double peak
- ✓ Five de-trapping energies 1.35 eV - 2.09 eV
- ✓ 3x higher D amount

Rate equation modelling (MHIMS, Hodille et al. JNM 2017)



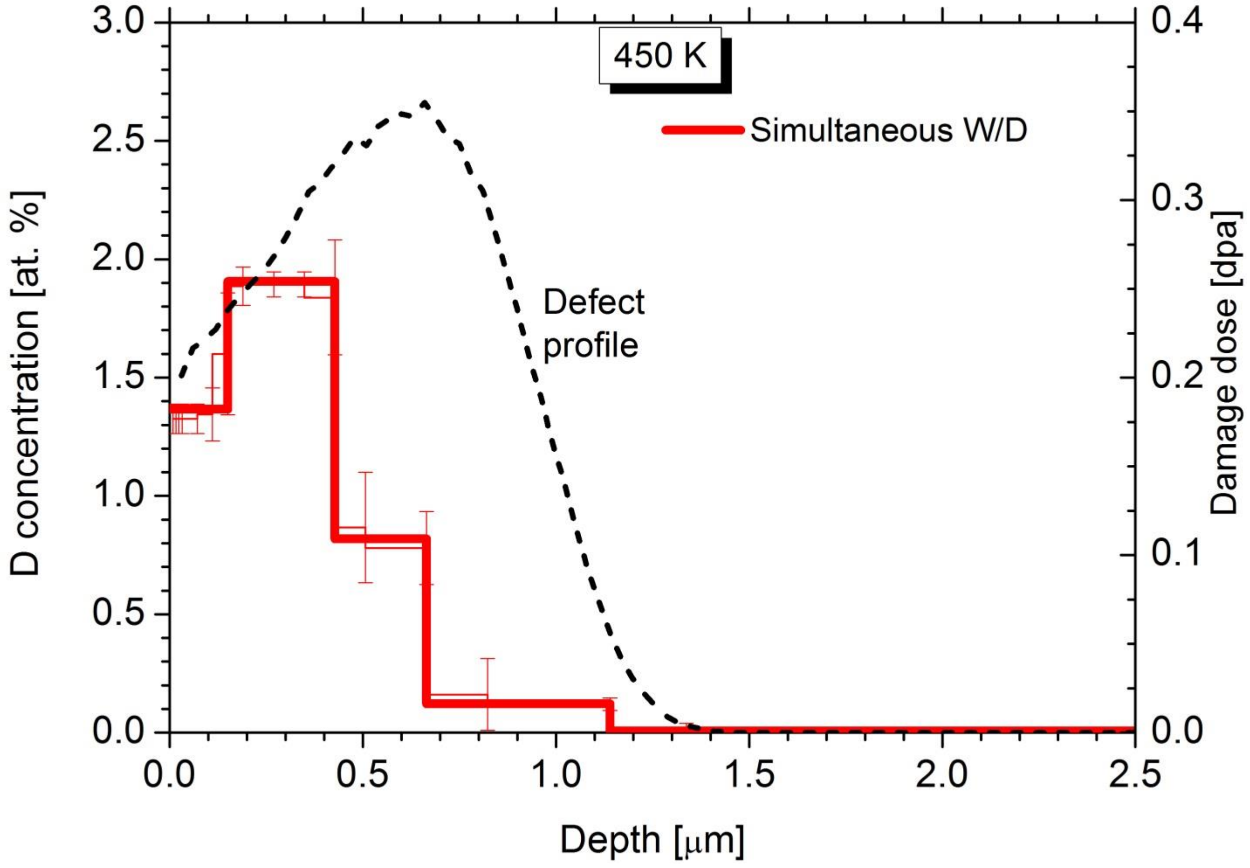
Simultaneous W/D exposure



Simultaneous W/D exposure:
W ion irradiation
D ion exposure
@ 450 K

4h simultaneous W/D
W ions – flux 9.73×10^{13} W/m^2s – 0.34 dpa
D ions - Ion flux=$1.4x10^{18}$ D/m^2s
Γ_D=$2.0x10^{22}$ D/m^2

Simultaneous W/D exposure @ 450 K
D depth profile



Simultaneous W/D-D exposure @ 450 K

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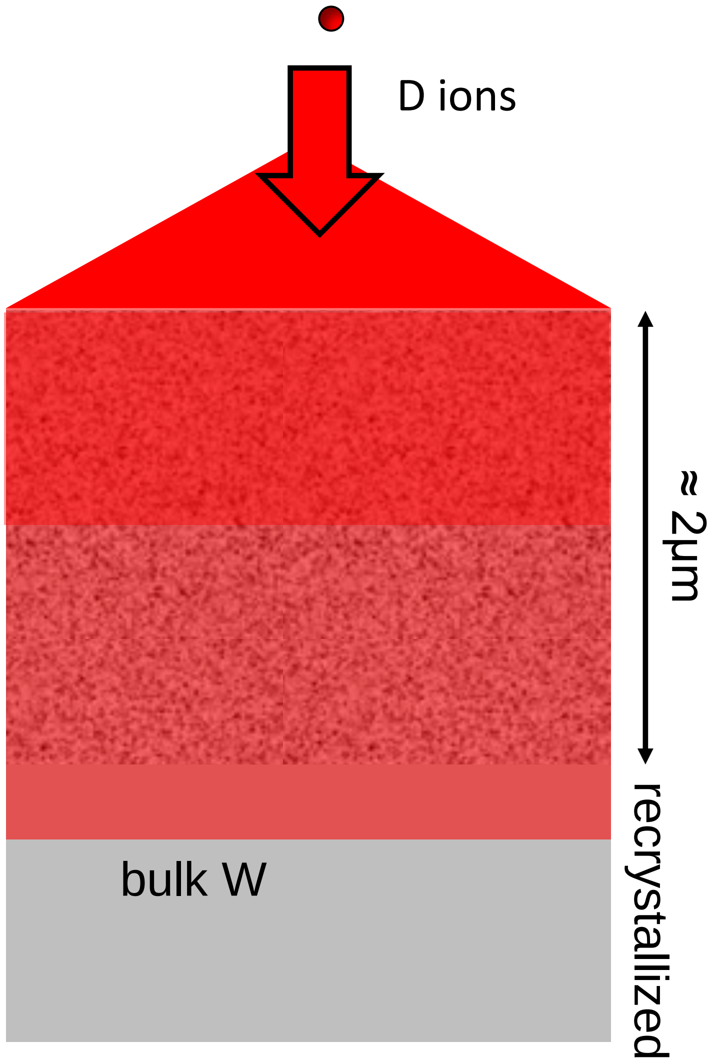


Simultaneous W/D-D exposure:

W ion irradiation @ 450 K

D ion exposure

+

D ion exposure @ 450 K – to populate created traps

4h simultaneous W/D

W ions – flux 9.73×10^{13} W/m²s – 0.34 dpa

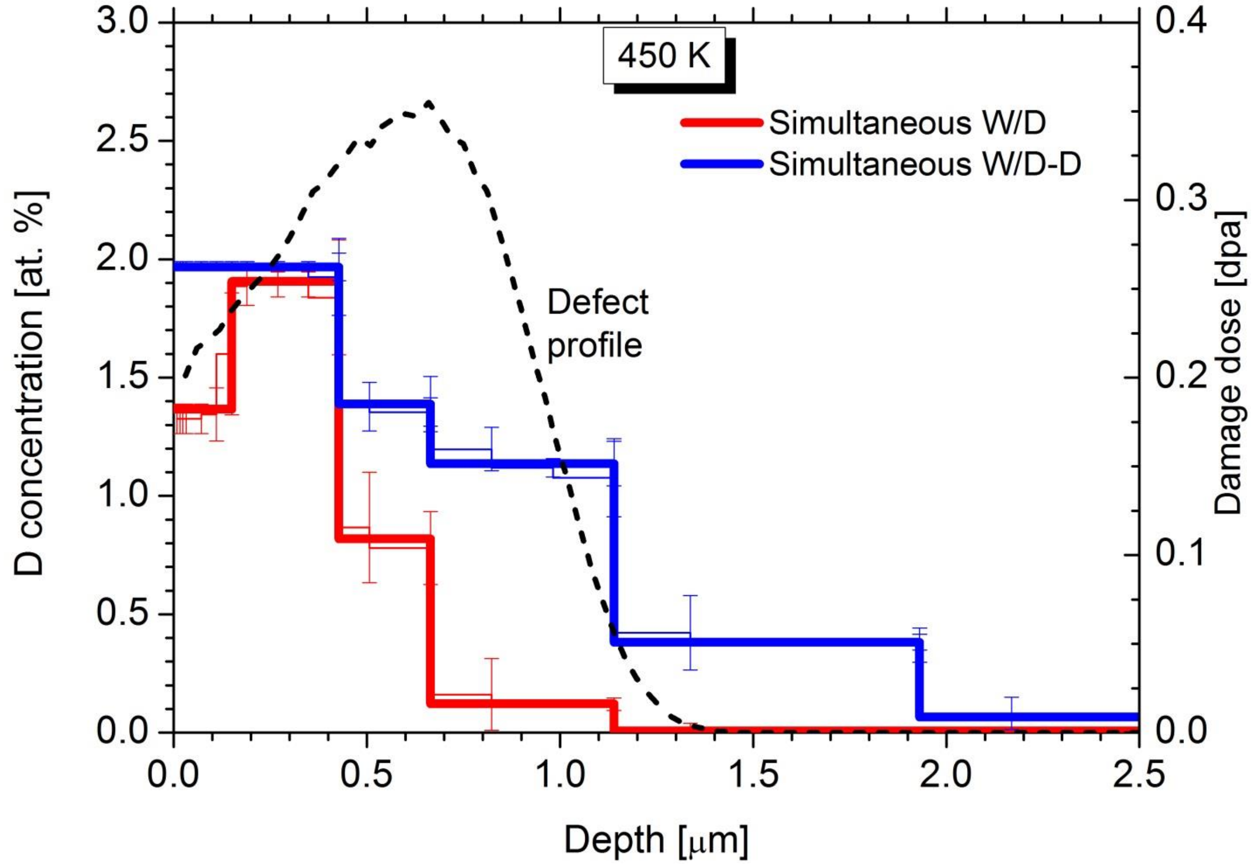
D ions - Ion flux=1.4x10^{18} D/m²s.

D fluence=2.0x10^{22} D/m²

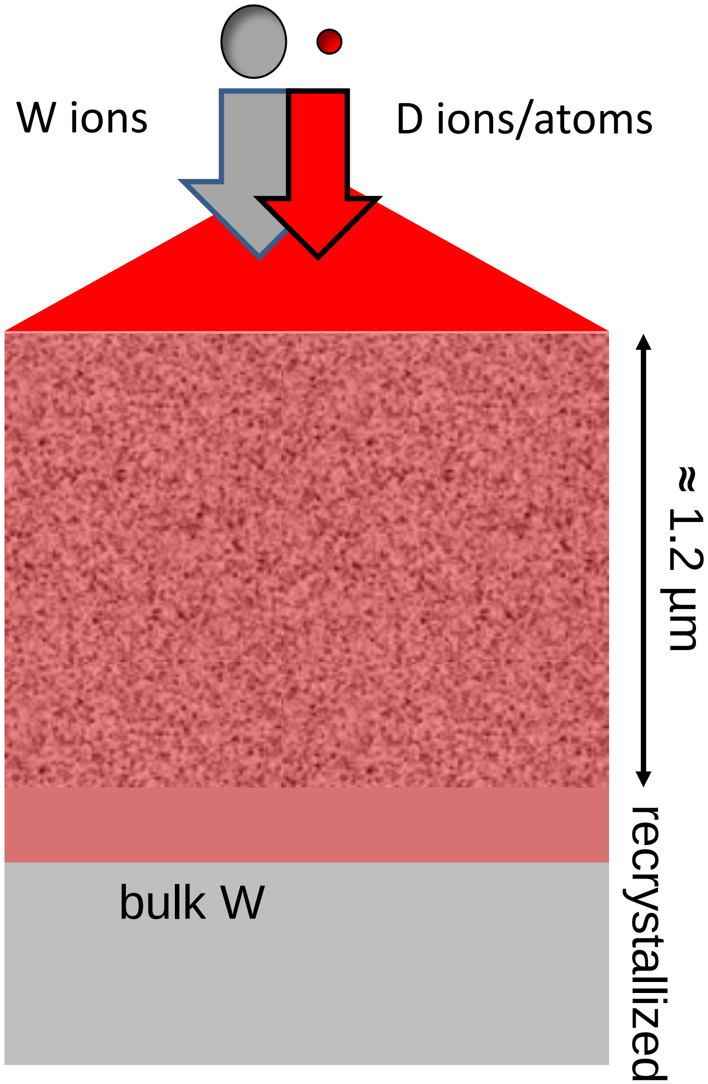
+

41h D ion exposure - D fluence 2.1×10^{23} D/m²

Simultaneous W/D-D exposure @ 450 K
D depth profile



Sequential W-D exposure



Sequential W-D exposure:

W ion irradiation **@ 450 K**

+

D ion exposure **@ 450 K to populate created traps**

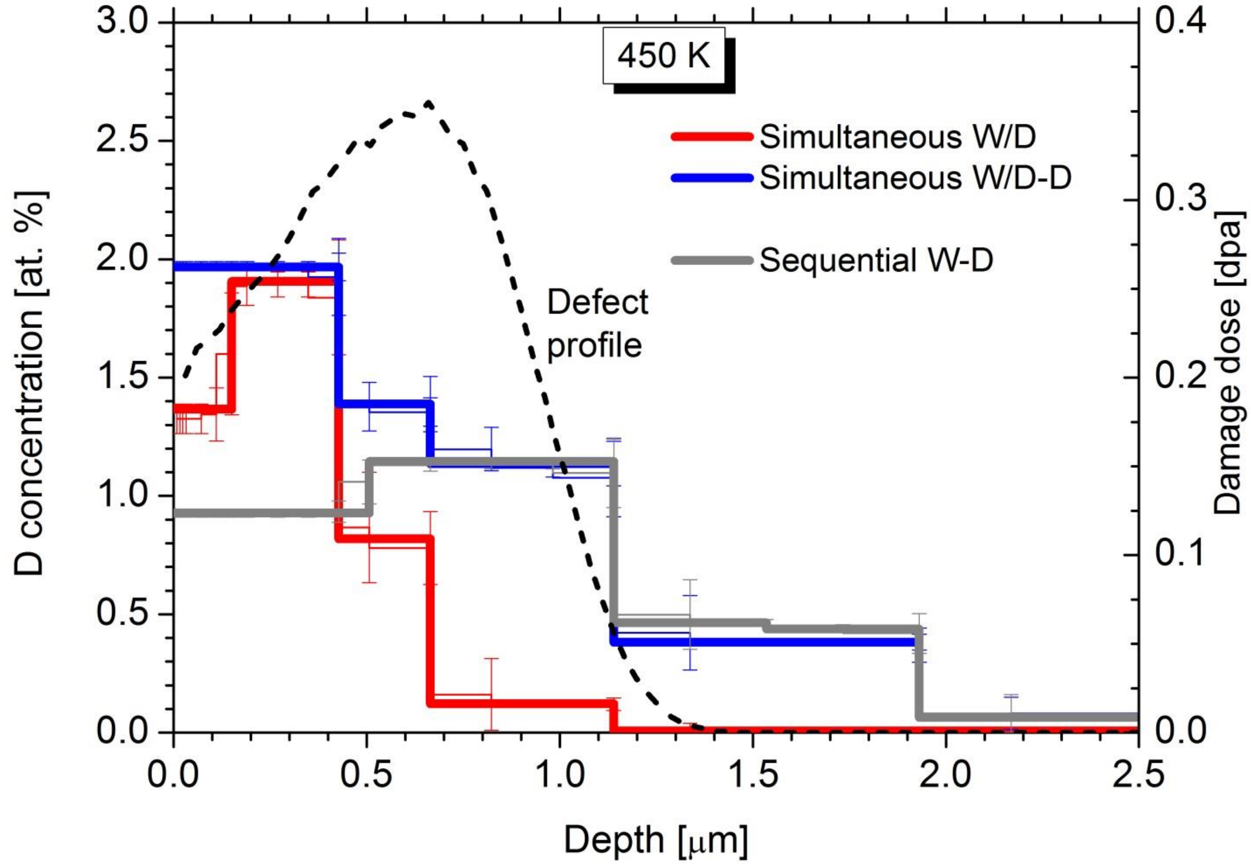
4h W irradiation

W ions – flux 9.73×10^{13} W/m²s – 0.34 dpa

+

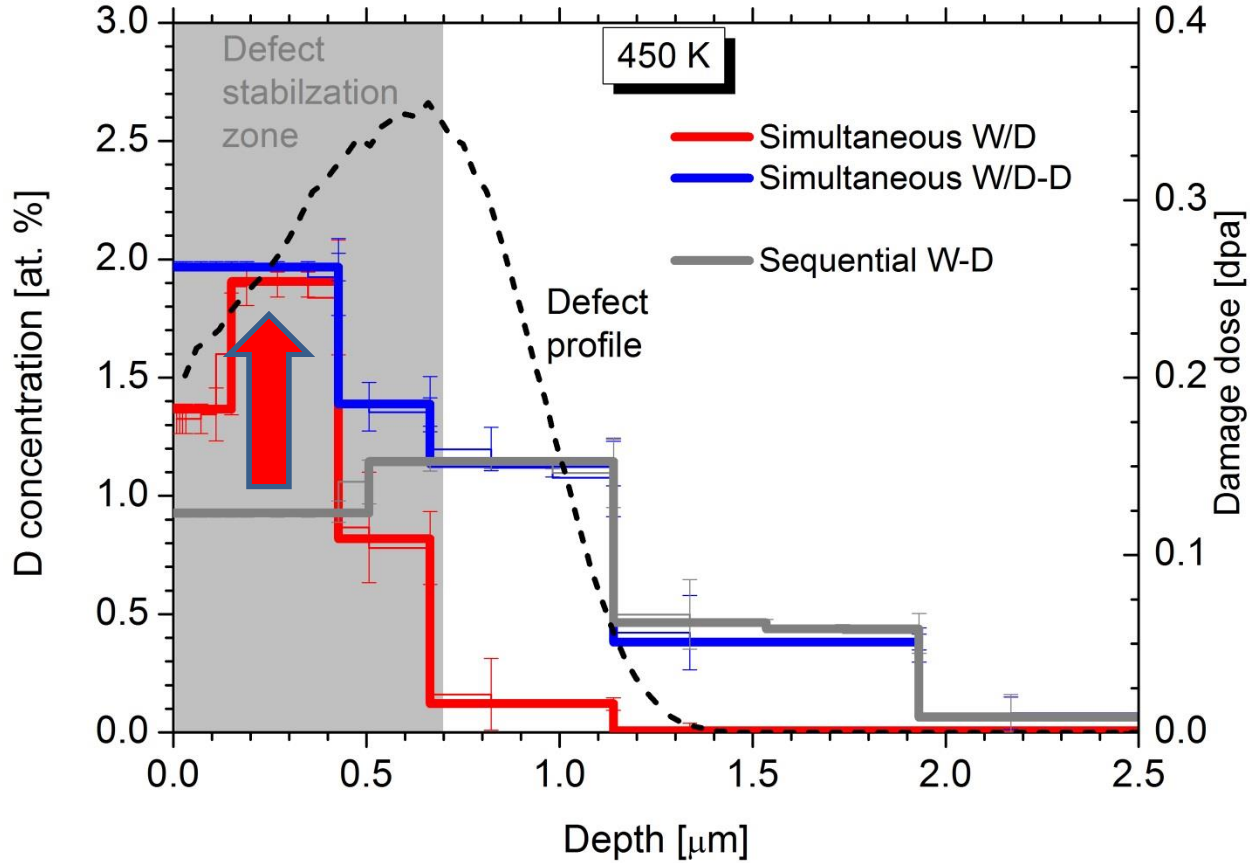
39 h D ion exposure - D fluence 2.0×10^{23} D/m²

D depth profile comparison @ 450 K



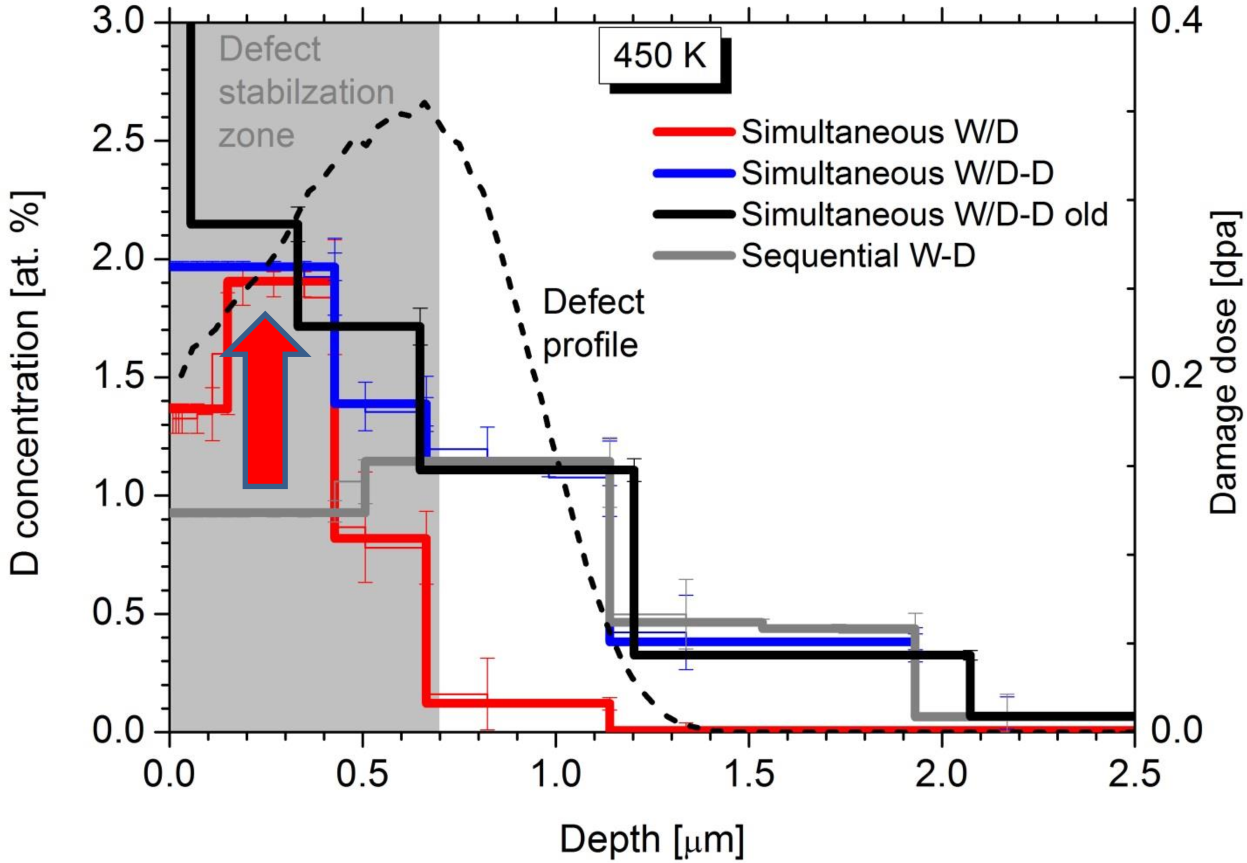
D depth profile comparison @ 450 K

- Difference in D concentration in the region where D was trapped during the 1. step – simultaneous W/D
- Factor of 2 difference



D depth profile comparison @ 450 K

- Difference in D concentration in the region where D was trapped during the 1. step – simultaneous W/D
- Factor of 2 difference
- Comparison to older measurement – D depth profile similar with stepped distribution

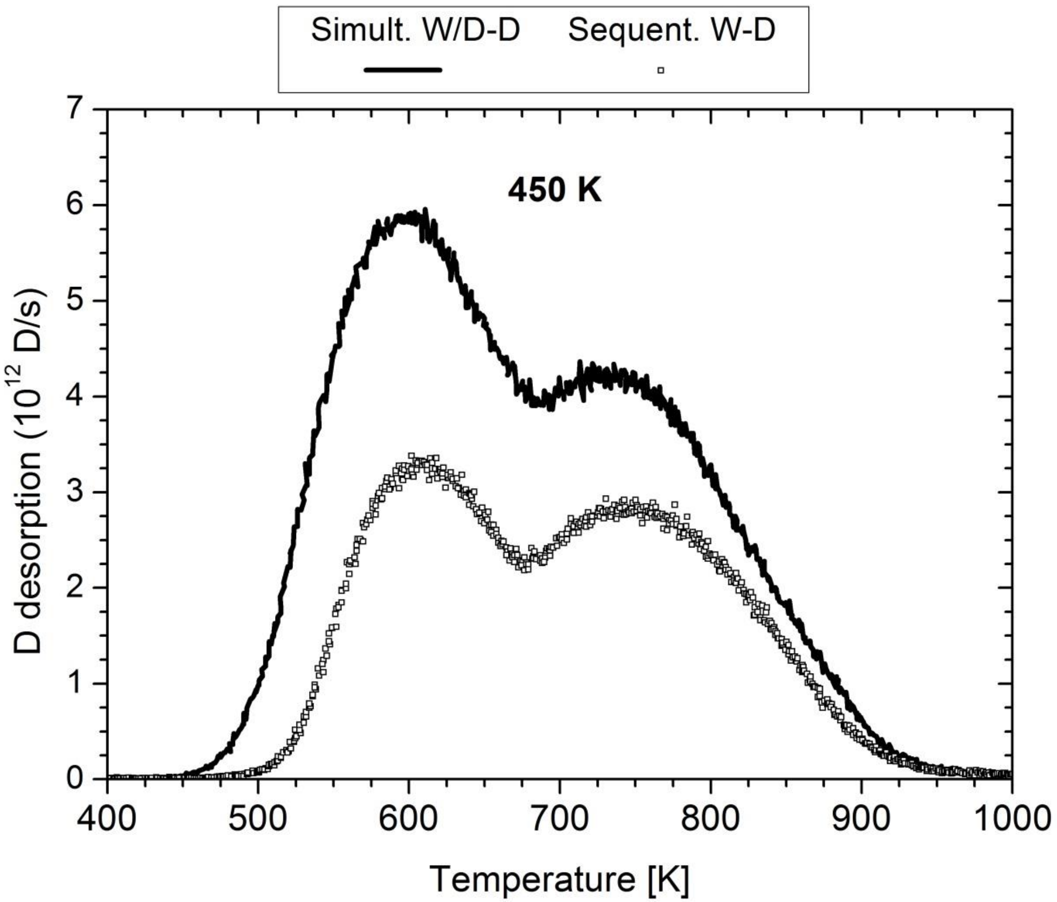


Comparison TDS sequential / simultaneous

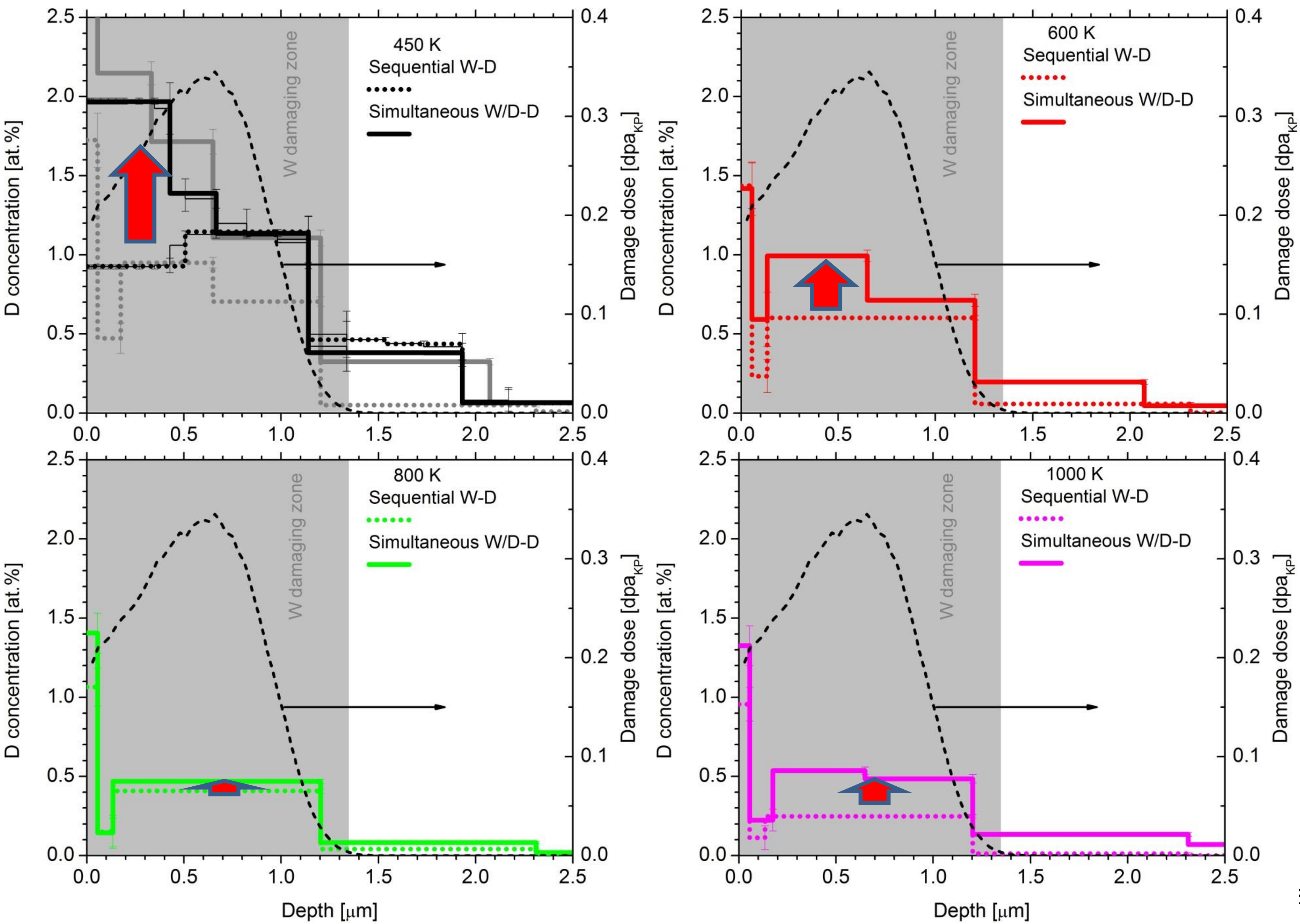
- Defect population by 300eV/D ion exposure at 450K

✓ No drastic change in TDS peak shape - double peak for both cases

✓ Temperature dependence also for individual traps



D depth profile comparison – all temperatures

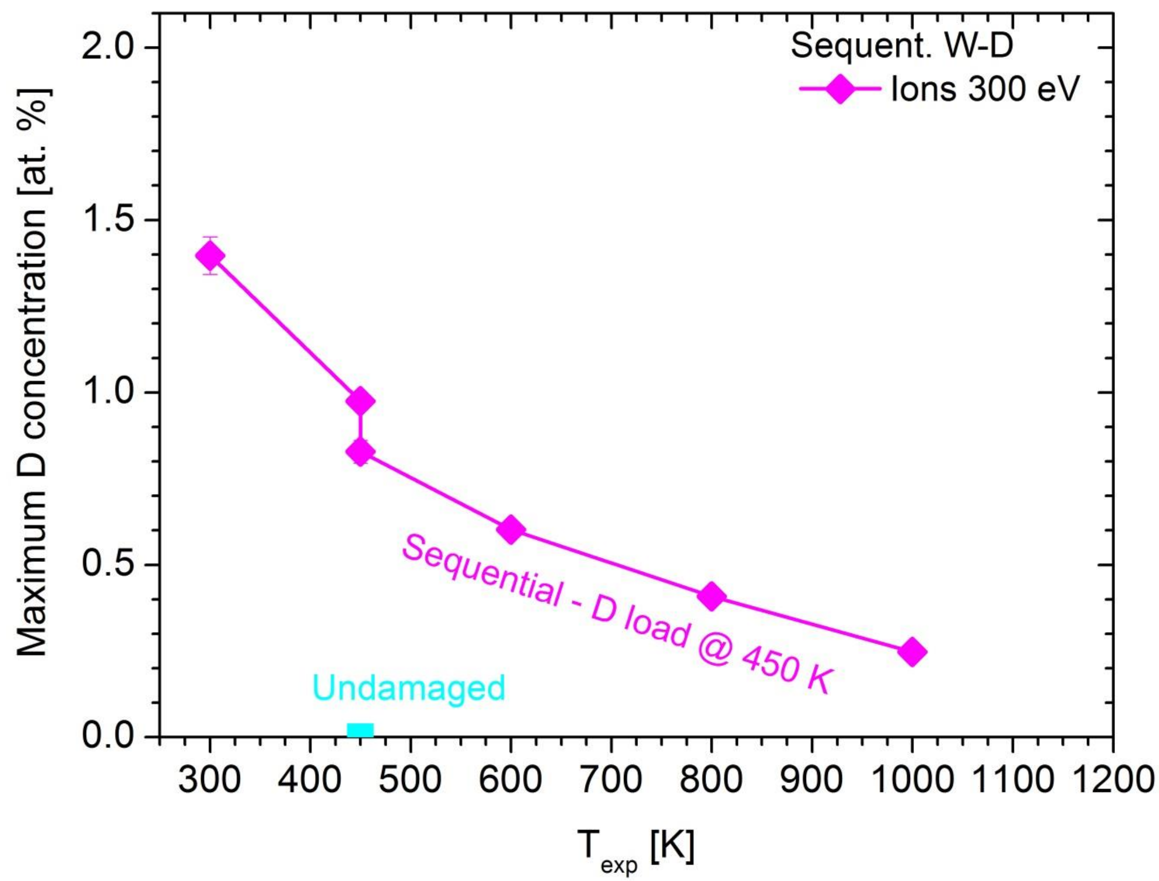


Sequential W-D exposure

- **Sequential W-D exposure**

- ✓ D concentration decreases with irradiation temperature
- ✓ Less defects created at elevated temperatures

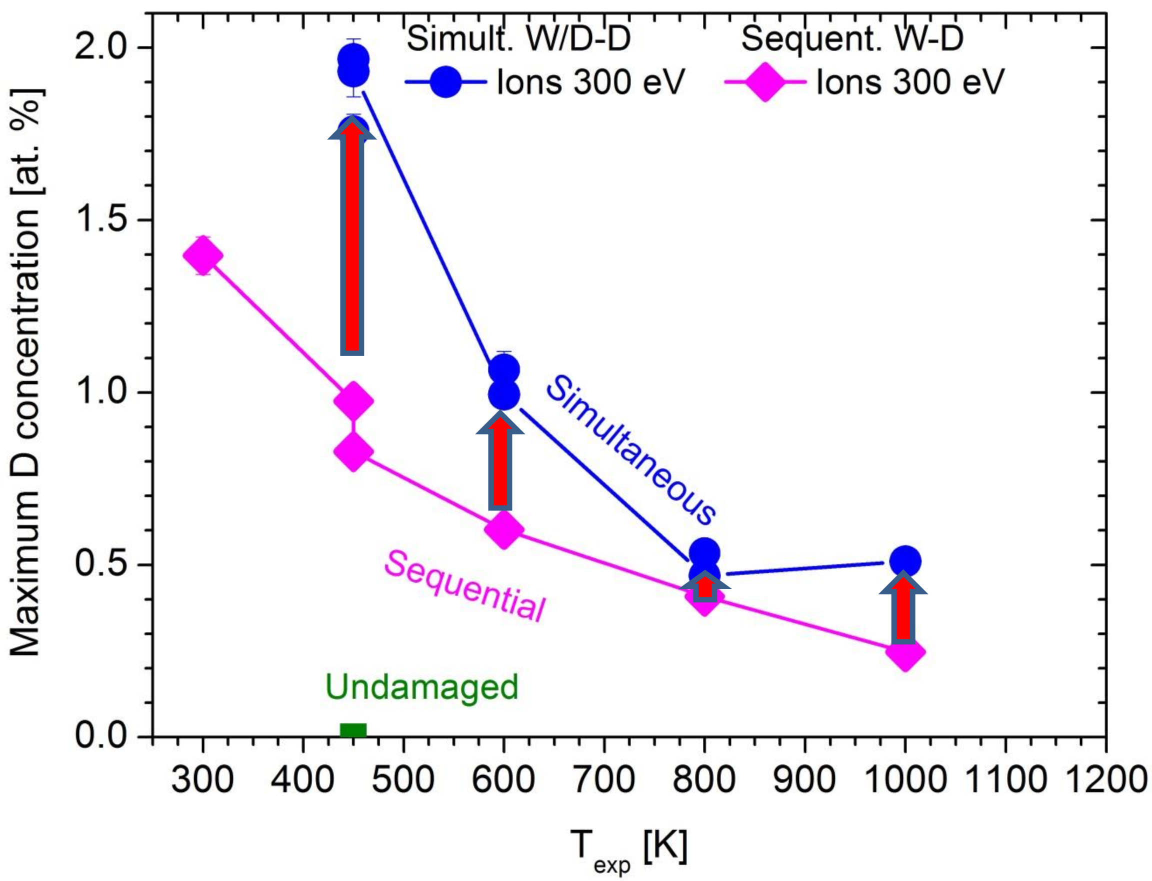
300 eV/D ion exposure at 450K



Comparison to Simultaneous W/D-D exposure

- **Sequential W-D exposure**
- **Simultaneous W/D-D exposure**
- Increase of D concentration – larger defect concentration
- Strong temperature dependence:
  - 450 K – 2.1
  - 600 K – 1.7
  - 800 K – 1.1
  - 1000 K – 2.1

300 eV/D ion exposure at 450K



Simultaneous W/D exposure
D depth profiles – all temperatures

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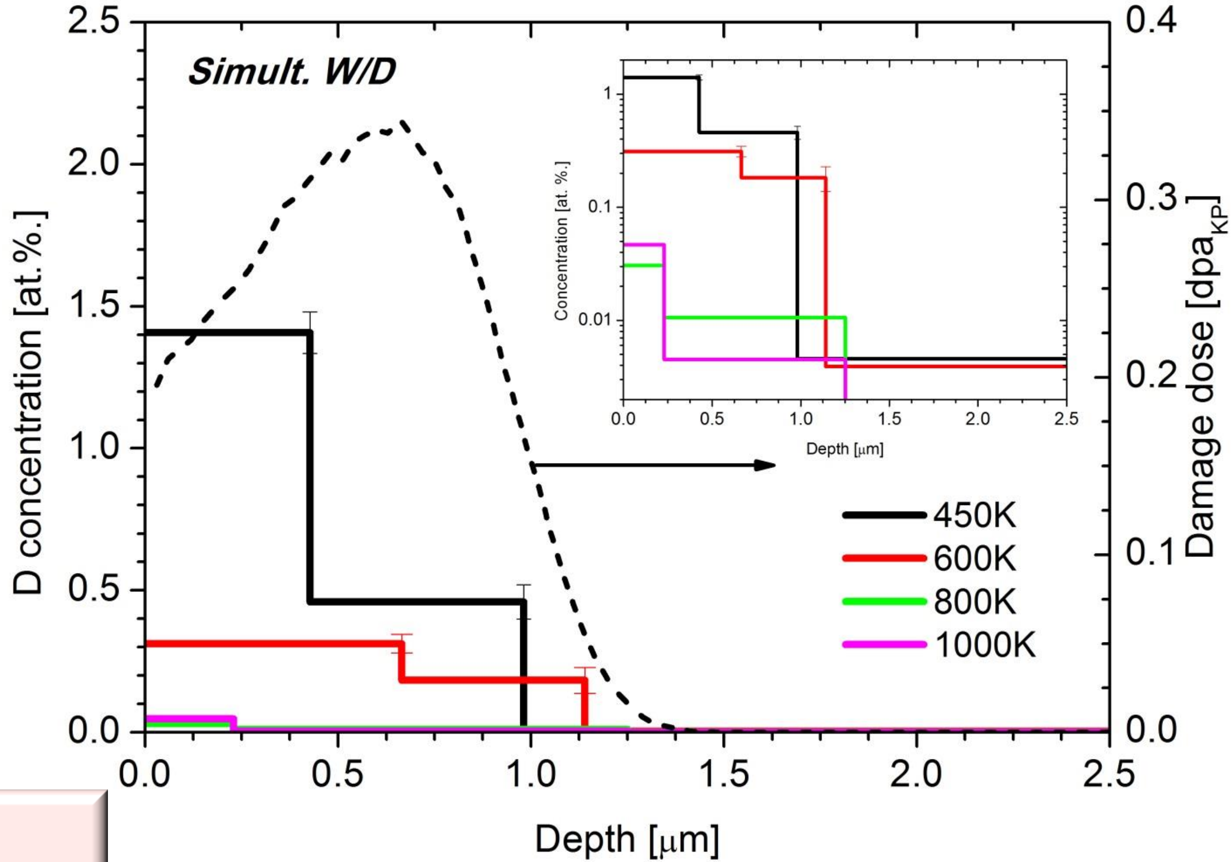
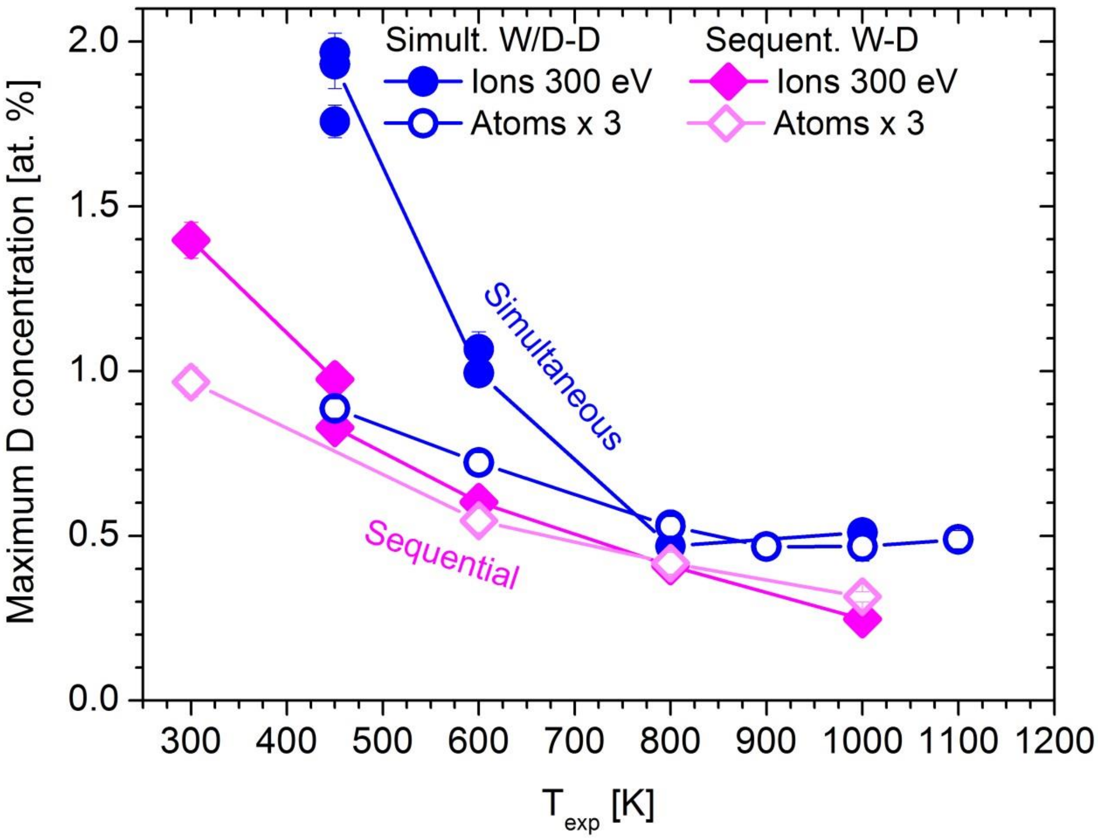
Simultaneous W/D exposure:

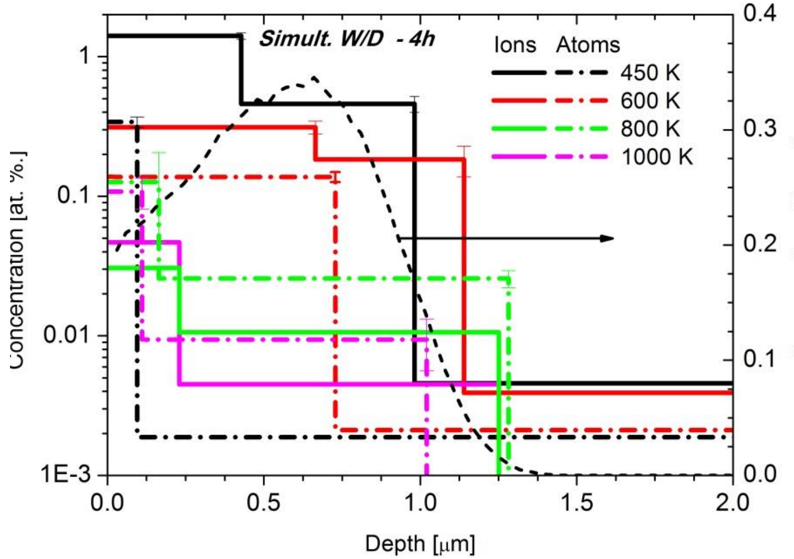
- ✓ Depth profiles after first 4h
- ➢ **Temperature determines the speed of diffusion and population of traps by D**
- ➢ **Lower D retention at high temperatures due to thermal D de-trapping**

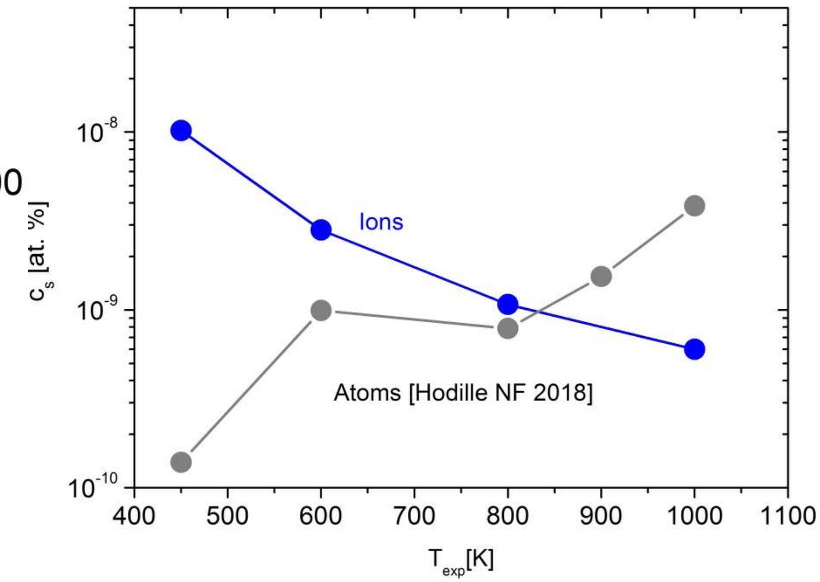


Defect stabilization dependent on the D concentration during the simultaneous W/D

Comparison ions versus atoms







- D concentration during W/D exposure determines the efficiency of defect stabilization by D presence

Effect of presence of D
Ab-initio calculations

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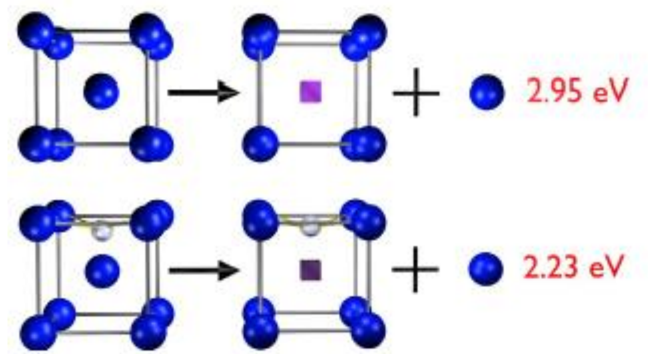
Fusion device scenario neutron irradiation during D/T plasma exposure

Two possible effects

Density Functional Theory (DFT) calculation with hydrogen in interstitial tetrahedral site in W [S.C. Middleburgh et al. , JNM 448 (2014) 270–275]:

- **25% lower than the vacancy formation energy in W without H.**

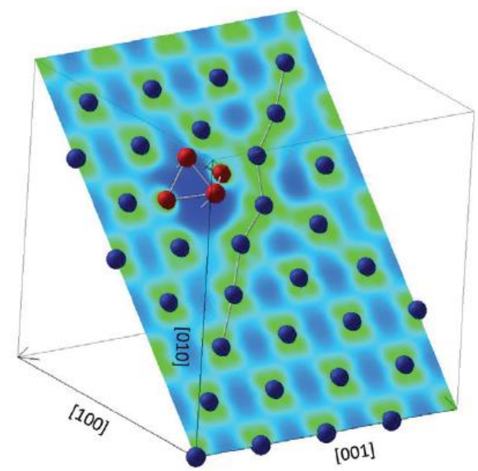
➢ **Higher probability of defect creation due to presence of H**



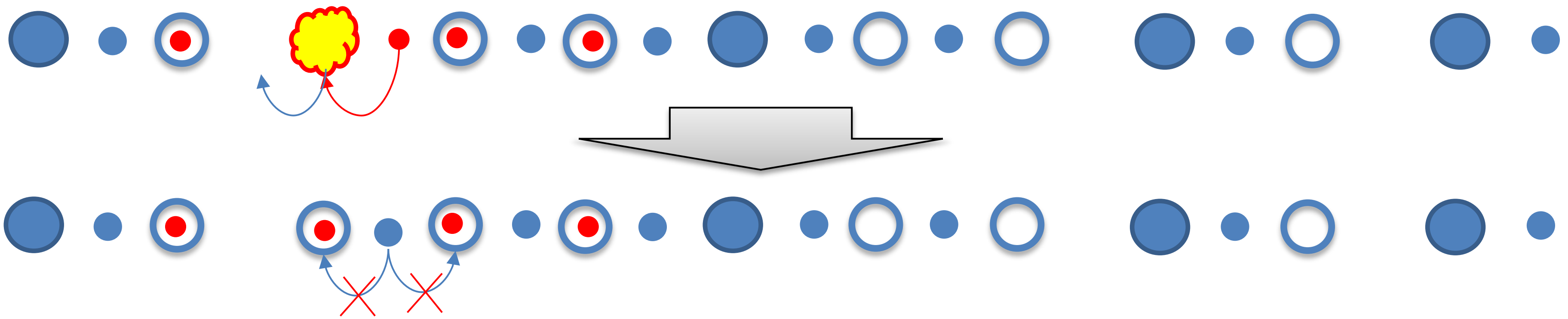
DFT calculation with hydrogen cluster in a vacancy in W [D. Kato et al. , NF **55** (2015) 083019]:

- Hydrogen cluster prevents vacancy from recombining with adjacent self-interstitial atoms (1 1 1-crowdion)

➢ **Lower probability for defect annihilation due to trapped D**



Stabilization by D trapping



We have upgraded the damage creation model, first introduced by Duesing *et al. 1969,* Ogorodnikov JAP 2008, Hodille NF 2018 - by including a stabilization mechanism:

$$\frac{dn_i(x,t)}{dt} = \frac{\Gamma\,\eta_i\,\theta(x)}{\rho}\left[1 - \frac{\mathrm{n_i}(x,t)}{\mathrm{n_{i,max}}}\left(1 - \alpha_i \frac{\mathrm{n_i}(x,t) - n_i^0(x,t)}{\mathrm{n_i}(x,t)}\right)\right]$$

Defects are stabilized to a degree by D trapped in them, meaning that the probability for a Frenkel pair annihilation is lower. Stabilization is parametrized by a free parameter denoted as α_i.

Γ ... W ion flux (W $m^{-2}s^{-1}$)
η ... Creation probability (m^{-1})
$\theta(x)$ ... SRIM dam. distribution (1)
$\mathrm{n_{i,max}}$ ... Saturation density (1 (at. fr.))

M. Pečovnik et al. under review in Nucl. Fusion

Experiment versus modelling

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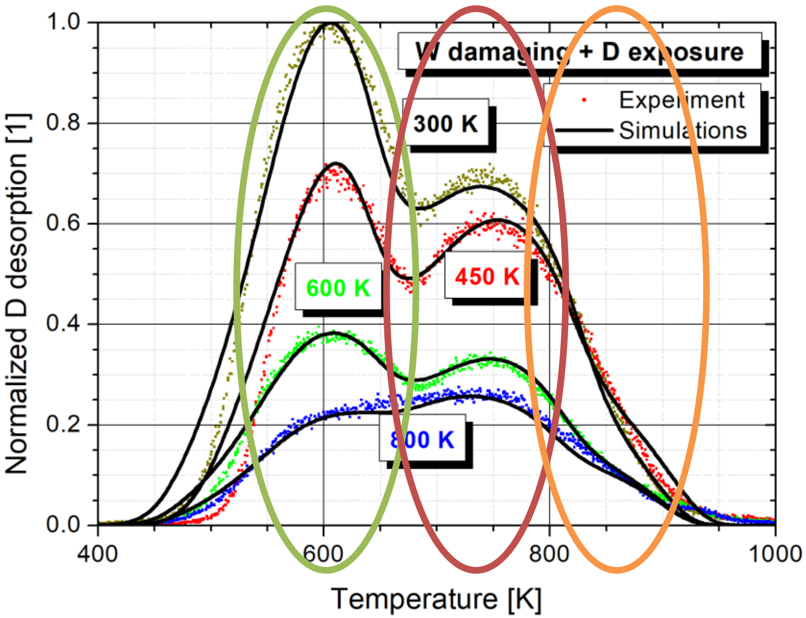
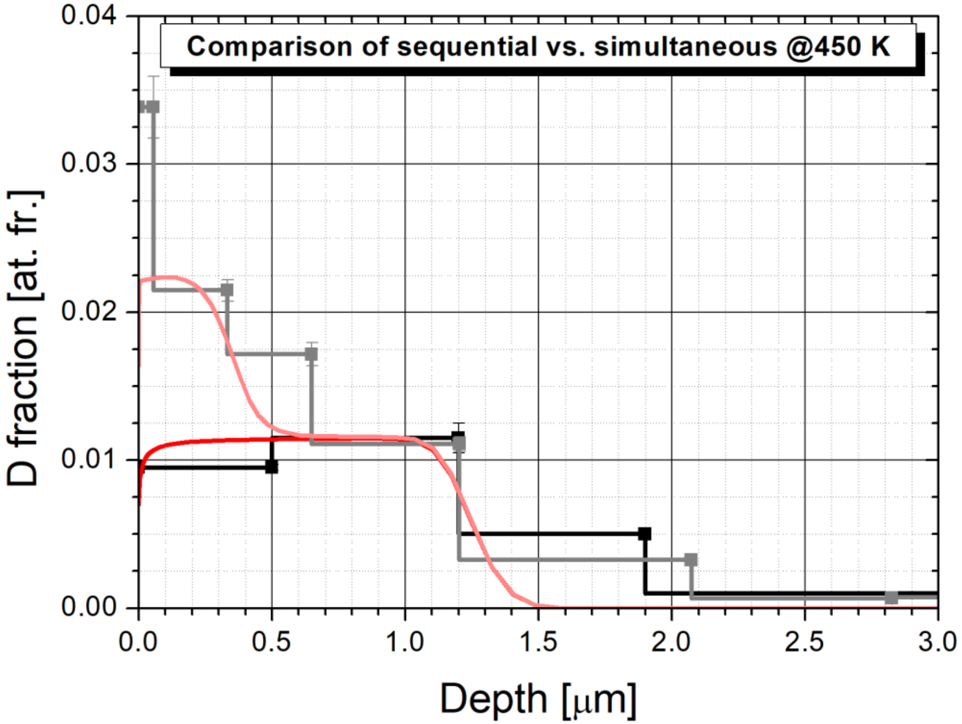
TDS



VACANCIES – 2 fill levels
S. VACANCY CLUSTERS – 2 fill levels
L. VACANCY CLUSTERS – 1 fill level

D depth profiles



Stabilization by trapped D

Conclusions

Study of D presence on displacement damage stabilization

Sequential W-D experiment

- **Decreased D retention with higher temperature**

Simultaneous W/D-D experiment

- **Effect of stabilization of defects increased for ion exposure as compared to atoms**
- **Observed temperature dependence of defect stabilization**
- **Concentration of created traps dependent on D concentration during the simultaneous W/D**
- **Increase of D concentration at 1000 K unclear**

- **Fusion scenario: higher fluxes of hydrogen fuel – higher D concentration at high temperatures – larger effect**

References - ions

- S. Markelj, et al, Nucl. Fusion (2019) in press
- M. Pečovnik et al. under review Nucl. Fusion

References atoms:

- S. Markelj, et al, Nuclear Materials and Energy 12 (2017) 169.
- E. Hodille et al. Nucl. Fusion **59** (2019) 016011

D mobile concentration comparison