



# Deuterium retention in self-ion irradiated tungsten: influence of irradiation temperature, damage dose, and alloying elements

M. Zibrov<sup>1</sup>, T. Schwarz-Selinger<sup>1</sup>, A. Cintora<sup>1</sup>, M. Klimenkov<sup>2</sup>

<sup>1</sup> Max Planck Institute for Plasma Physics, Garching, Germany

<sup>2</sup> Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

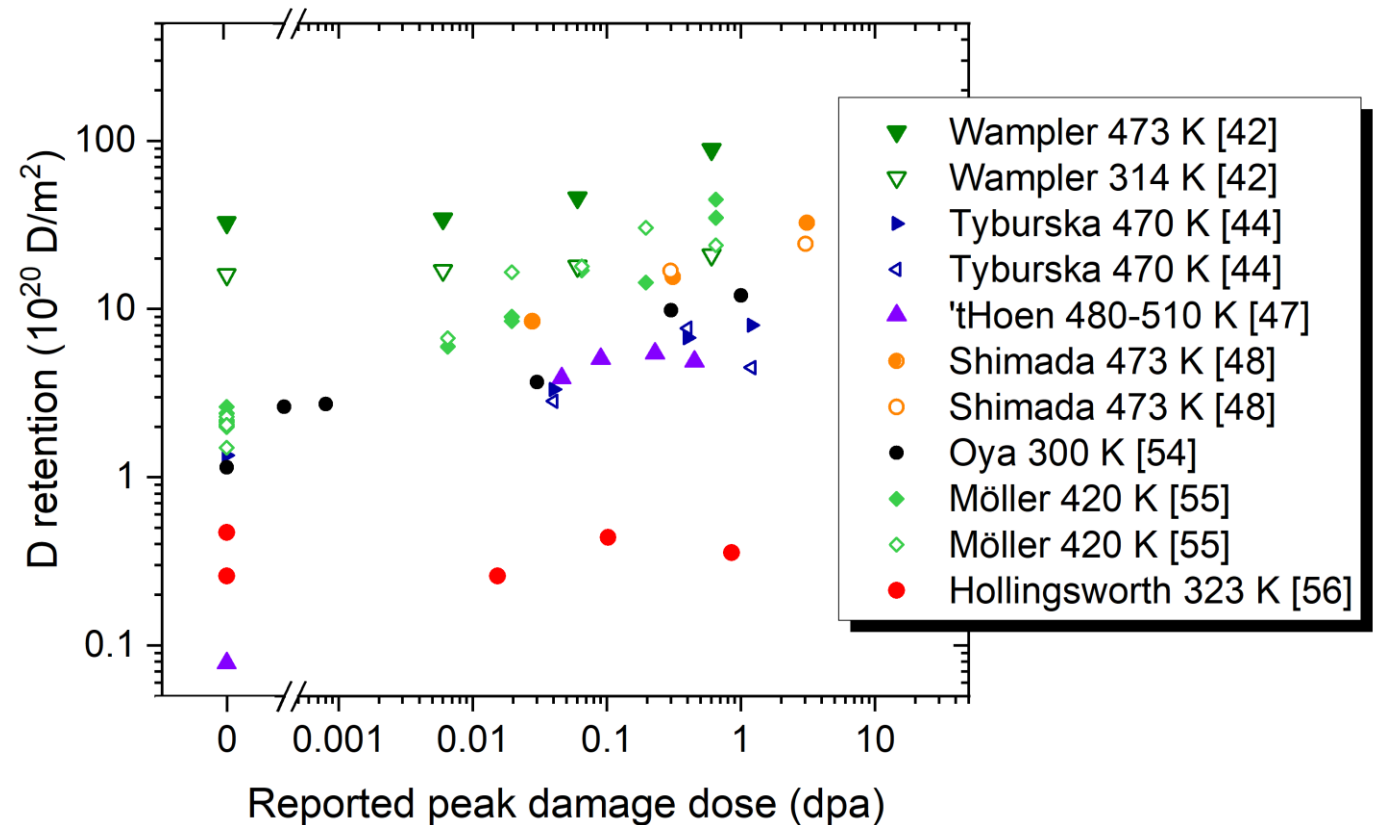




# Motivation: Evolution of D retention in W with damage dose displacement-damaging at room temperature

## *MeV ion irradiation to simulate displacement damage produced by fusion neutrons*

- D retention scatters
- Typically very limited dpa range
- ⇒ Total retention values of little use (TDS)
- ⇒ Possible defect creation during D loading



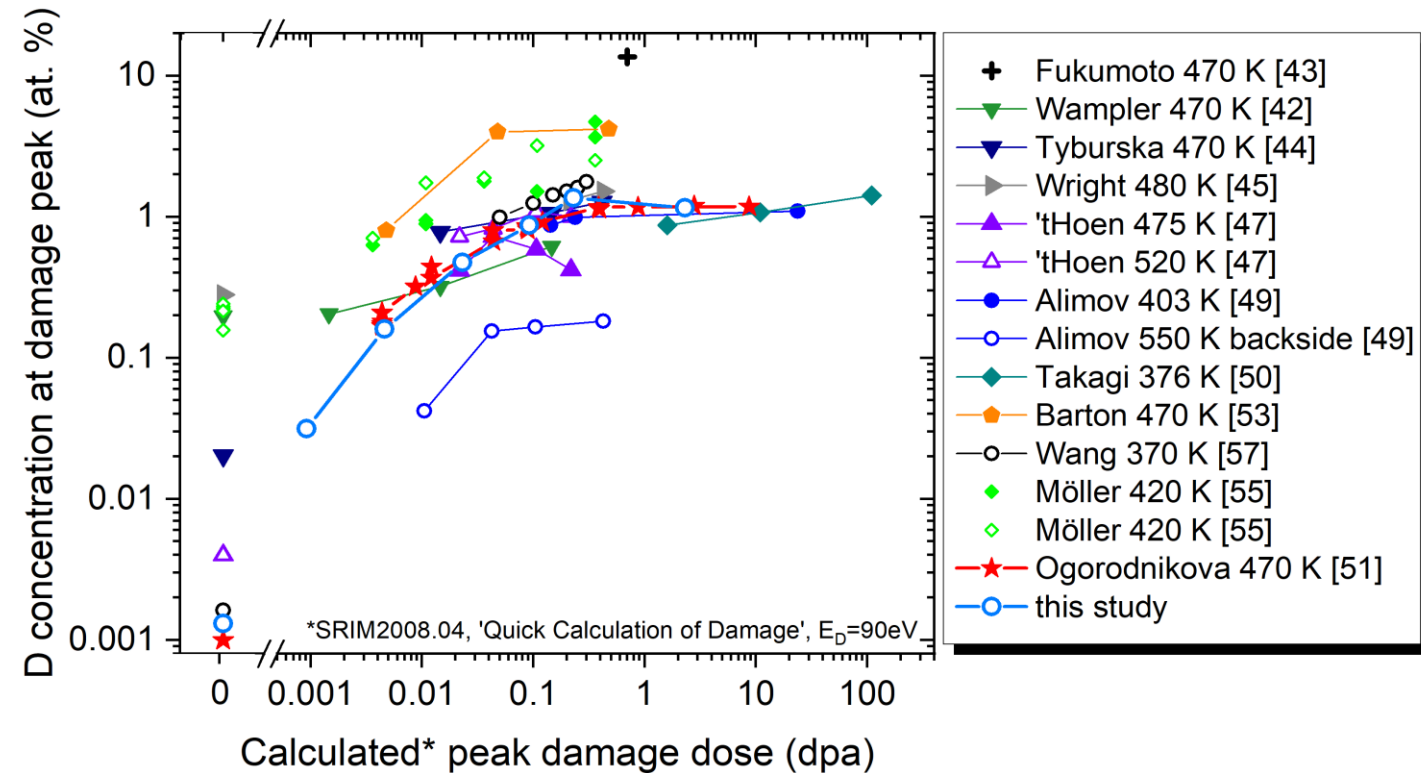
T. Schwarz-Selinger, Mater. Res. Express 10, 102002 (2023).



# Motivation: Evolution of D retention in W with damage dose displacement-damaging at room temperature

## MeV ion irradiation to simulate displacement damage produced by fusion neutrons

- D retention scatters
- Typically very limited dpa range
- ⇒ Total retention values of little use (TDS)
- ⇒ Possible defect creation during D loading
- ⇒ Absolute D concentrations necessary (GD-OES, NRA)



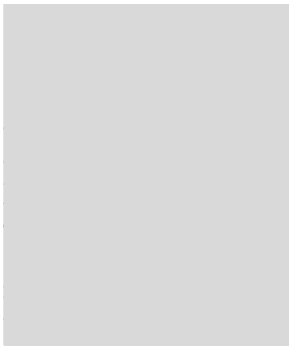


# Experimental methodology

## 1. 'Defect-free' samples

2000 K annealed W (10-50  $\mu\text{m}$  grain size)

Polycryst. W





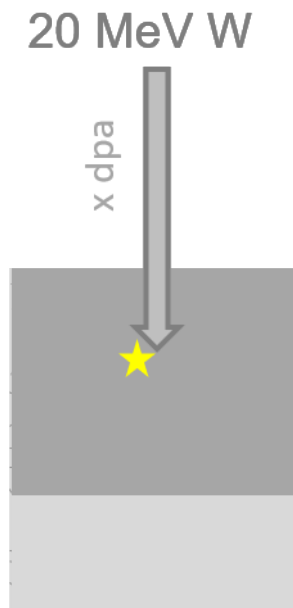
# Experimental methodology

## 1. 'Defect-free' samples

2000 K annealed W (10-50  $\mu\text{m}$  grain size)

## 2. Creating displacement damage

20 MeV W ion irradiation



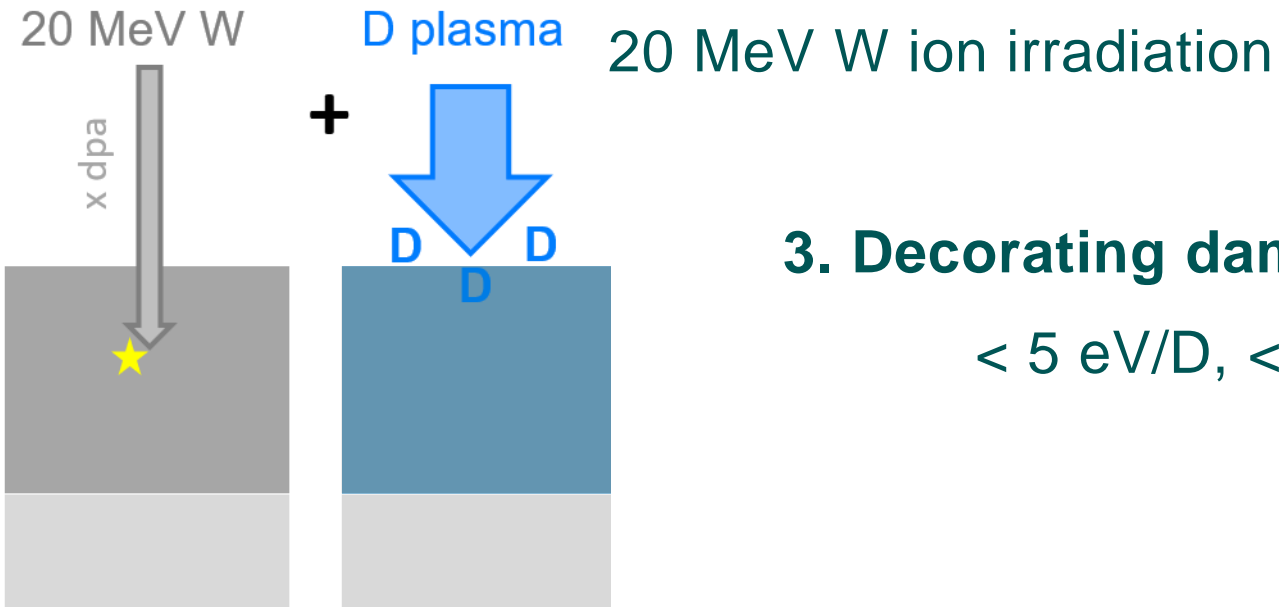


# Experimental methodology

## 1. 'Defect-free' samples

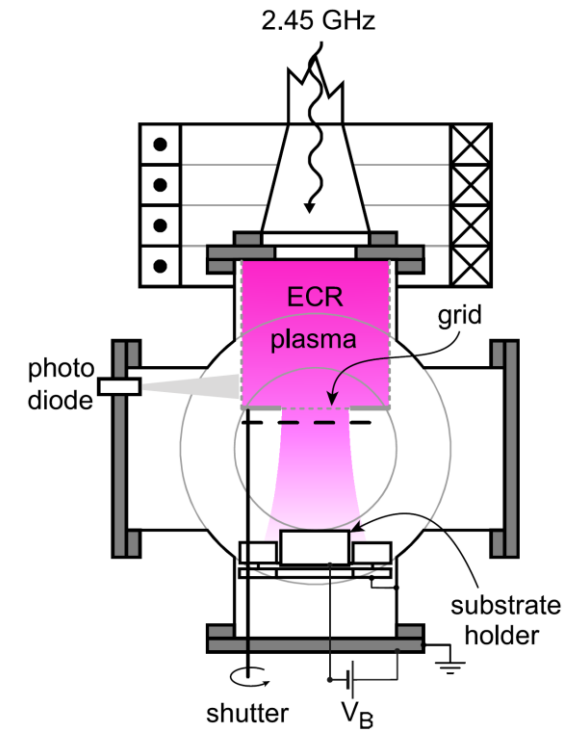
2000 K annealed W (10-50  $\mu\text{m}$  grain size)

## 2. Creating displacement damage



## 3. Decorating damage with deuterium

$< 5 \text{ eV/D}$ ,  $< 10^{20} \text{ D/m}^2\text{s}$ , 370 K,  $> 10^{25} \text{ D/m}^2$

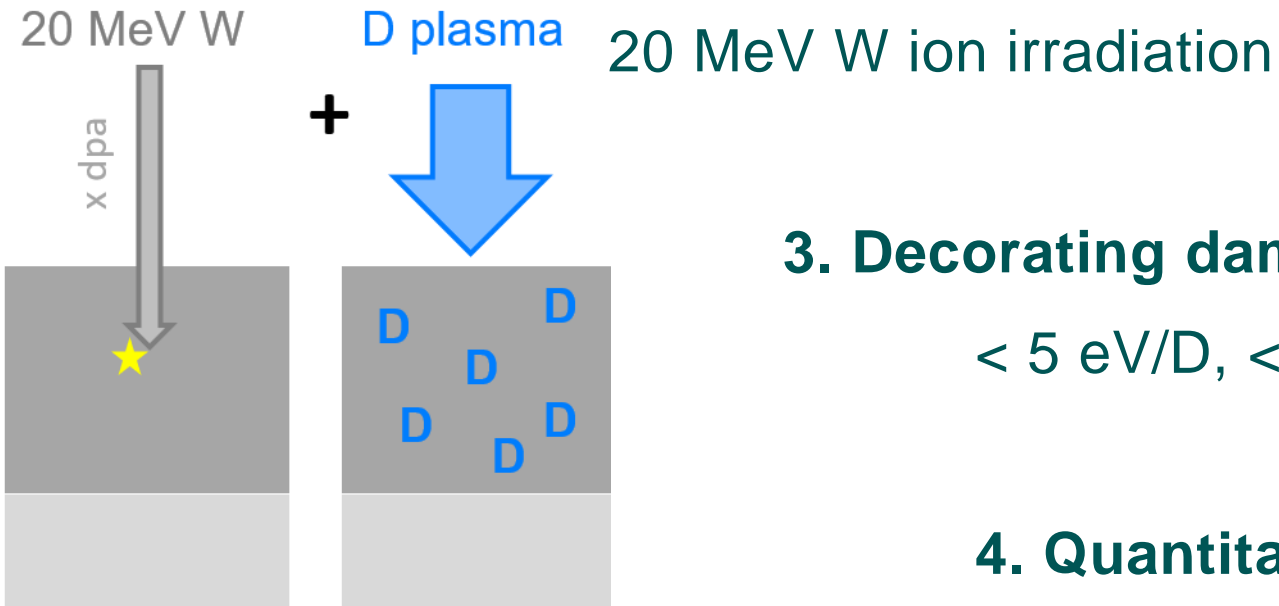


# Experimental methodology

## 1. 'Defect-free' samples

2000 K annealed W (10-50  $\mu\text{m}$  grain size)

## 2. Creating displacement damage

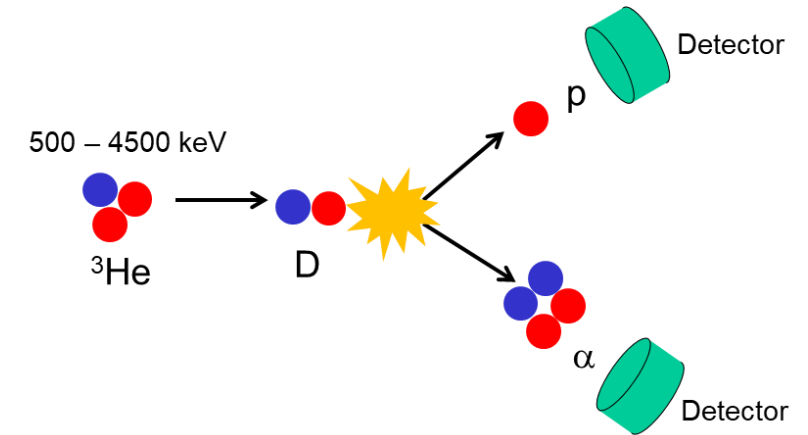


## 3. Decorating damage with deuterium

$< 5 \text{ eV/D}$ ,  $< 10^{20} \text{ D/m}^2\text{s}$ , 370 K,  $> 10^{25} \text{ D/m}^2$

## 4. Quantitative analyses

$\text{D}({}^3\text{He},\text{p})\alpha$  NRA depth profiling / TDS

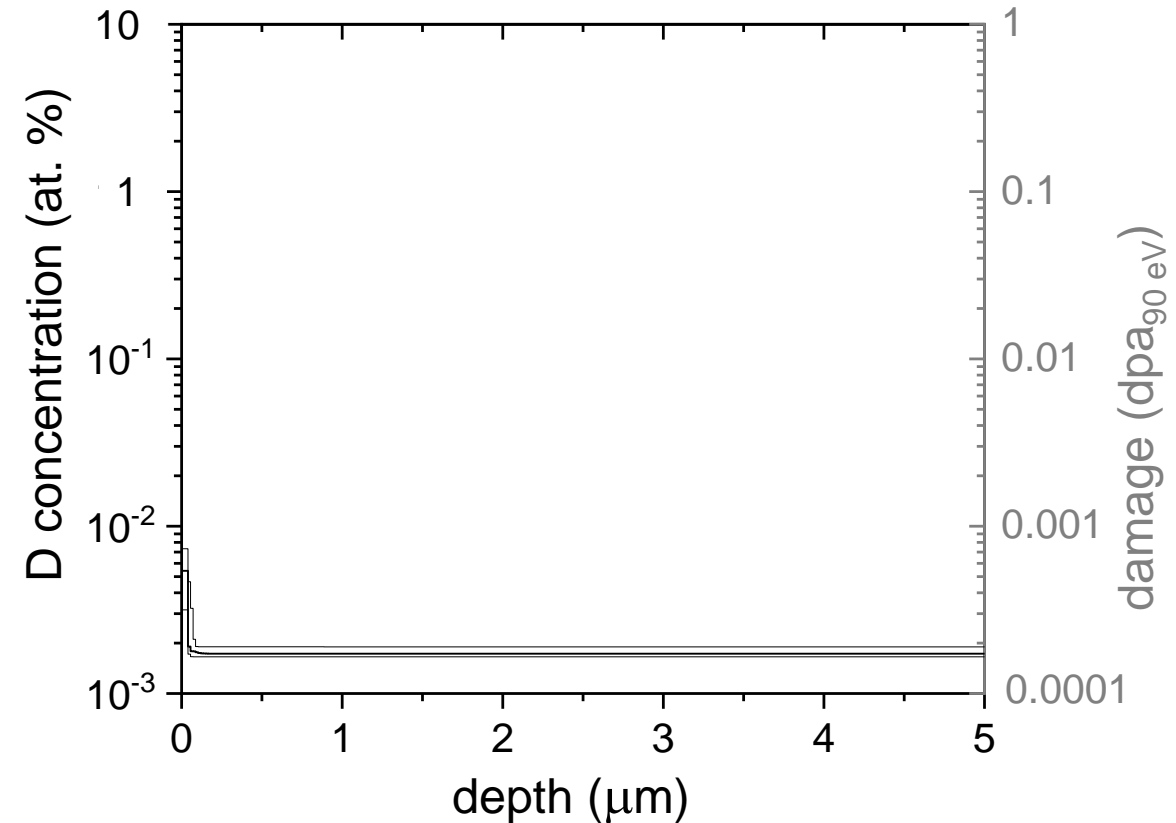




# Evolution of D retention in W with damage dose displacement-damaging at room temperature

**370 K gentle plasma exposure of recrystallized W for 72 h /  $1.5 \times 10^{25}$  D/m<sup>2</sup>**

- ⇒ Plasma exposure does not create defects
- ⇒ But only decorates the existing defects



T. Schwarz-Selinger et al., unpublished





# Evolution of D retention in W with damage dose displacement-damaging at room temperature

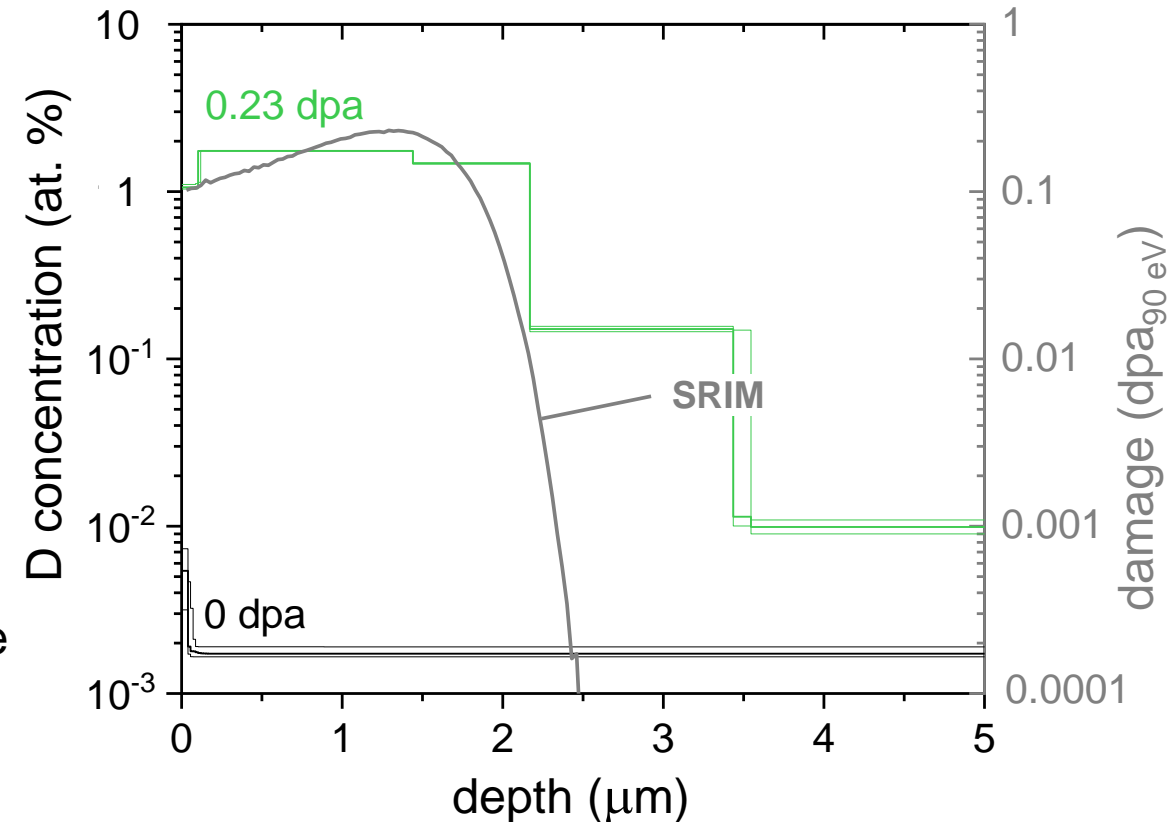
**370 K gentle plasma exposure of recrystallized W for 72 h /  $1.5 \times 10^{25}$  D/m<sup>2</sup>**

- ⇒ Plasma exposure does not create defects
- ⇒ But only decorates the existing defects

**Same plasma exposure of 20 MeV W-irradiated W (0.23 dpa)**

- + D retention increases by three orders of magnitude
- + D depth coincides with damage depth

⇒ **Methodology valid to study evolution of defect densities**

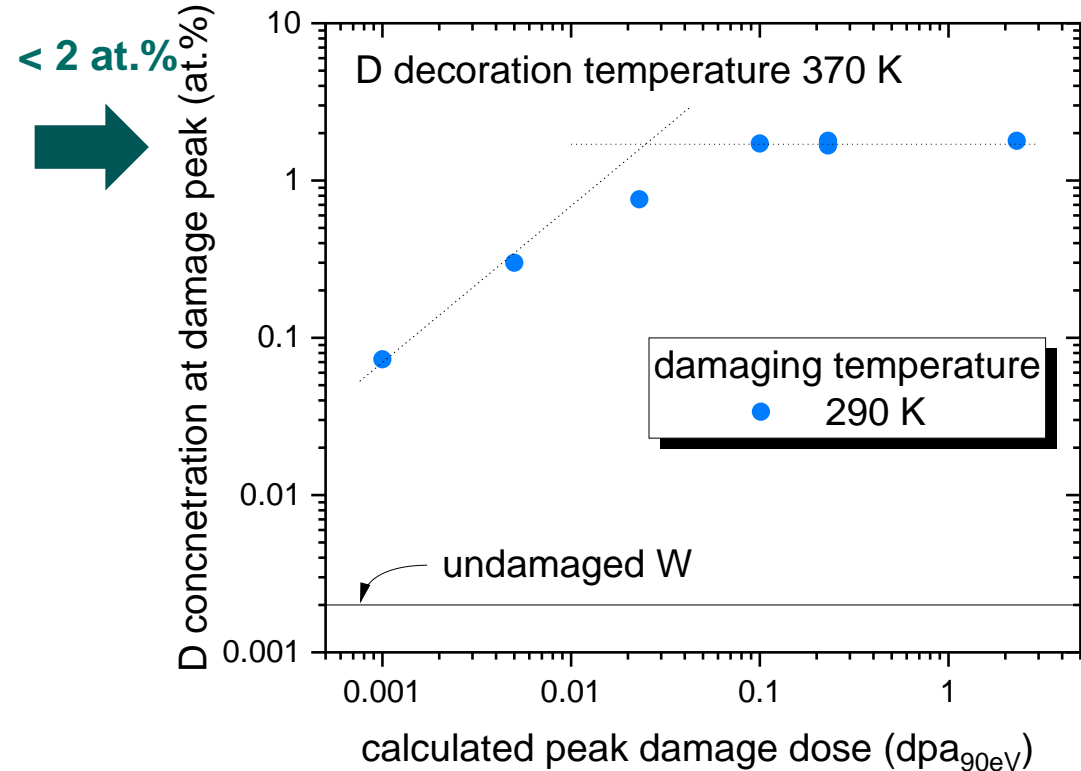




# Evolution of D retention in W with damage dose displacement-damaging at room temperature

## Experimental observations:

- $D_{\max} \propto \text{dpa}$  in the milli-dpa range
- Starts to deviate around 10 milli-dpa
- Reaches saturation value above 0.1 dpa
- $D_{\max} = 1.7 \text{ at.}\%$  for damaging at 290 K, i.e. 3 orders of magnitude above pristine W





# Comparison with modelling displacement-damaging at room temperature

***D.R. Mason et al., Phys. Rev. Mater. 5 (2021) 095403:***

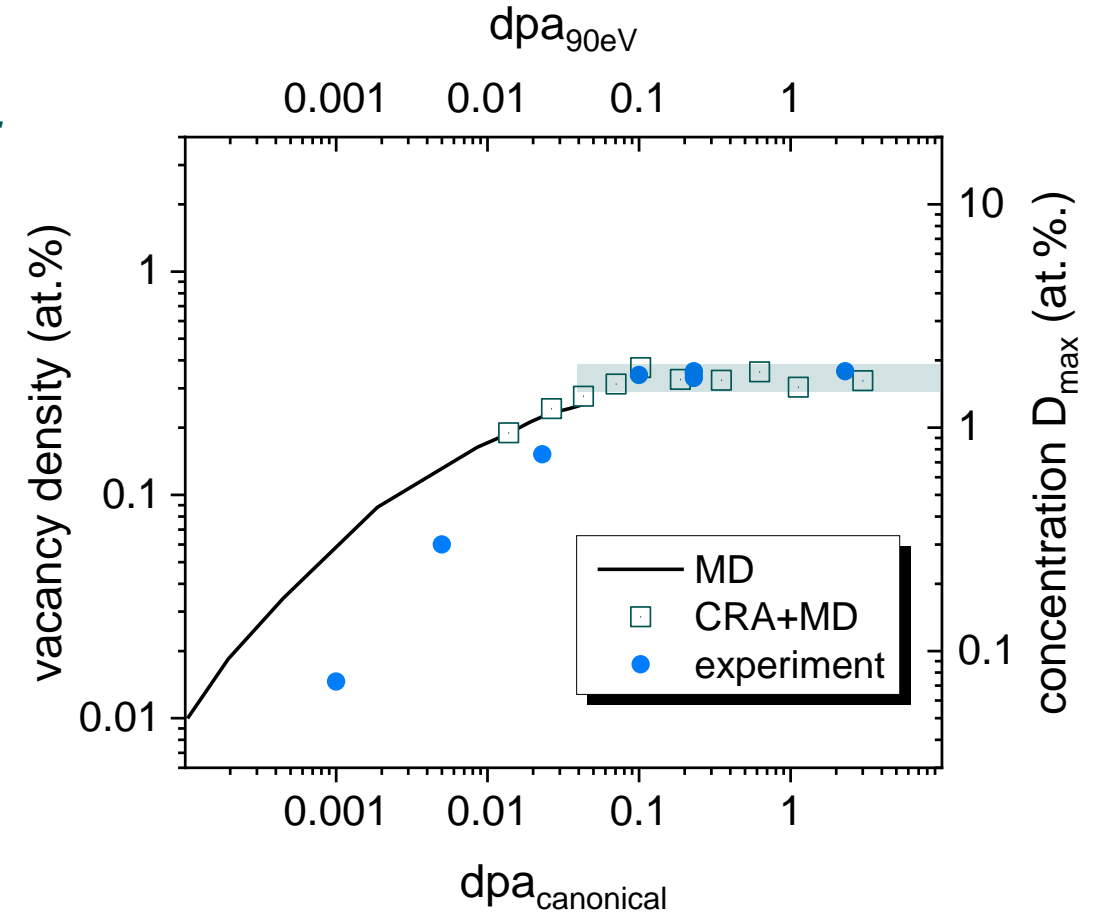
- Parameter-free modelling
- Assuming five D atoms per vacancy gives:  
 $D_{\max} = 1.5 - 2.0$  at.%

**Perfect match with present experiments in terms of:**

- Saturation behavior
- Absolute concentration  $D_{\max}$

**But: Damaging at room temperature**

**What about DEMO-relevant temperatures?**



MD: Molecular Dynamics

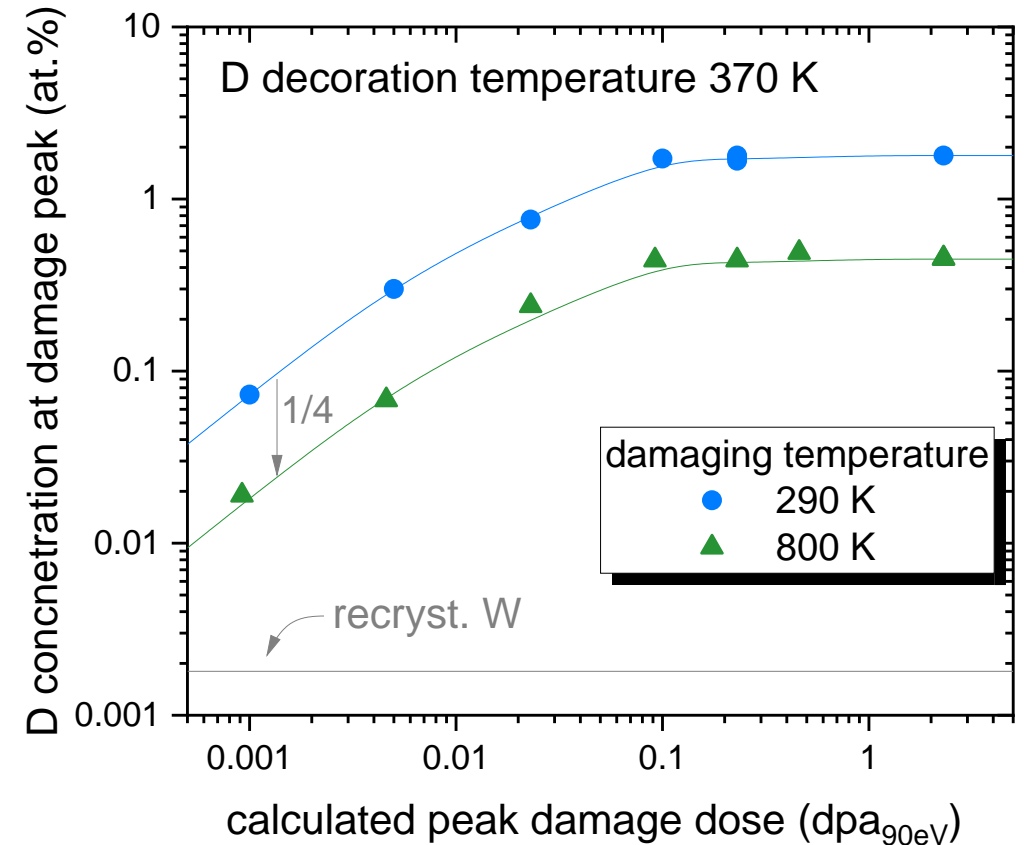
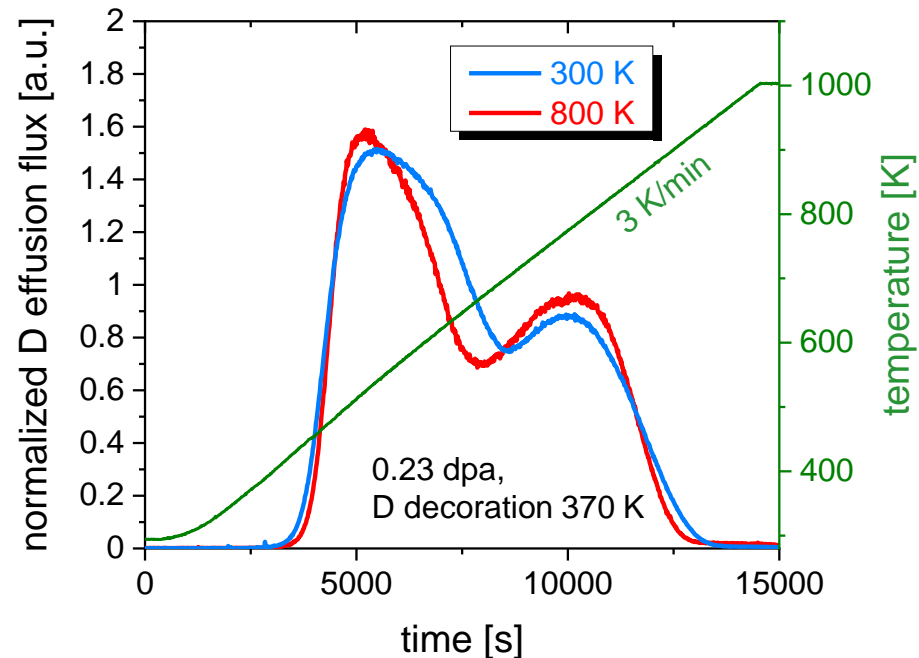
CRA: Creation Relaxation Algorithm



# Evolution of D retention in W with damage dose displacement-damaging at elevated temperature

## 800 K:

- Similar dependence on dpa as for 290 K
- $D_{\max}$  is 4 times smaller compared with 290 K
- TDS spectra shape similar as for 290 K



T. Schwarz-Selinger et al., unpublished



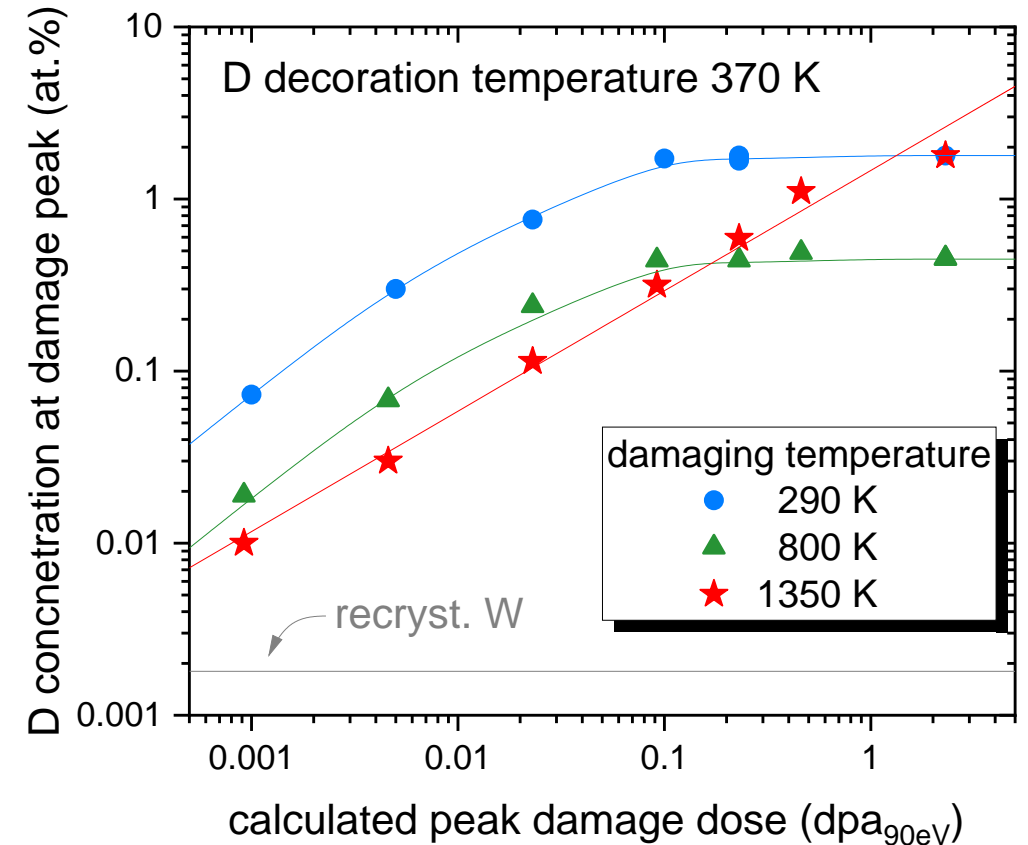
# Evolution of D retention in W with damage dose displacement-damaging at elevated temperature

## 800 K:

- Similar dependence on dpa as for 290 K
- $D_{\max}$  is 4 times smaller compared with 290 K
- TDS spectra shape similar as for 290 K

## 1350 K:

- No saturation yet
- $D_{\max} = 1.8$  at.% at 2.3 dpa!



T. Schwarz-Selinger et al., unpublished



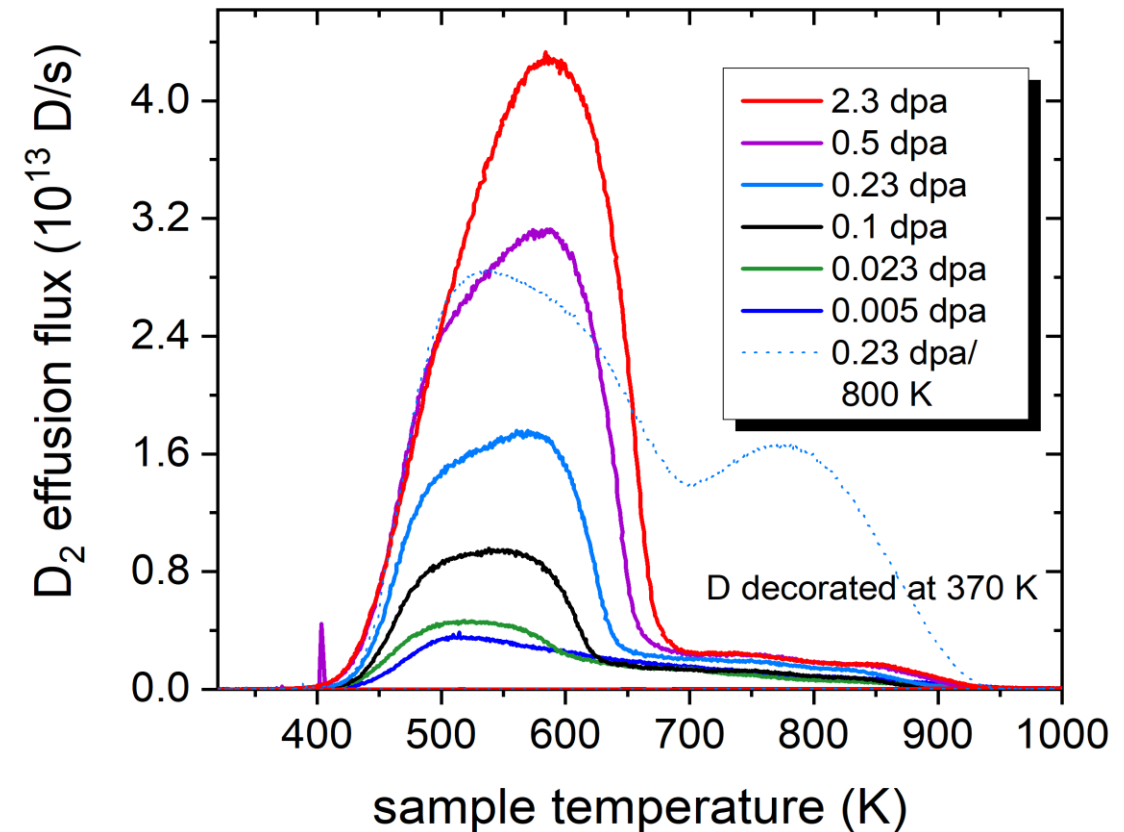
# Evolution of D retention in W with damage dose displacement-damaging at elevated temperature

## 800 K:

- Similar dependence on dpa as for 290 K
- $D_{\max}$  is 4 times smaller compared with 290 K
- TDS spectra shape similar as for 290 K

## 1350 K:

- No saturation yet
- $D_{\max} = 1.8$  at.% at 2.3 dpa!
- Different TDS spectra compared with 290 and 800 K
- **Change of defect type?**



T. Schwarz-Selinger et al., unpublished



# Evolution of D retention in W with damage dose displacement-damaging at elevated temperature

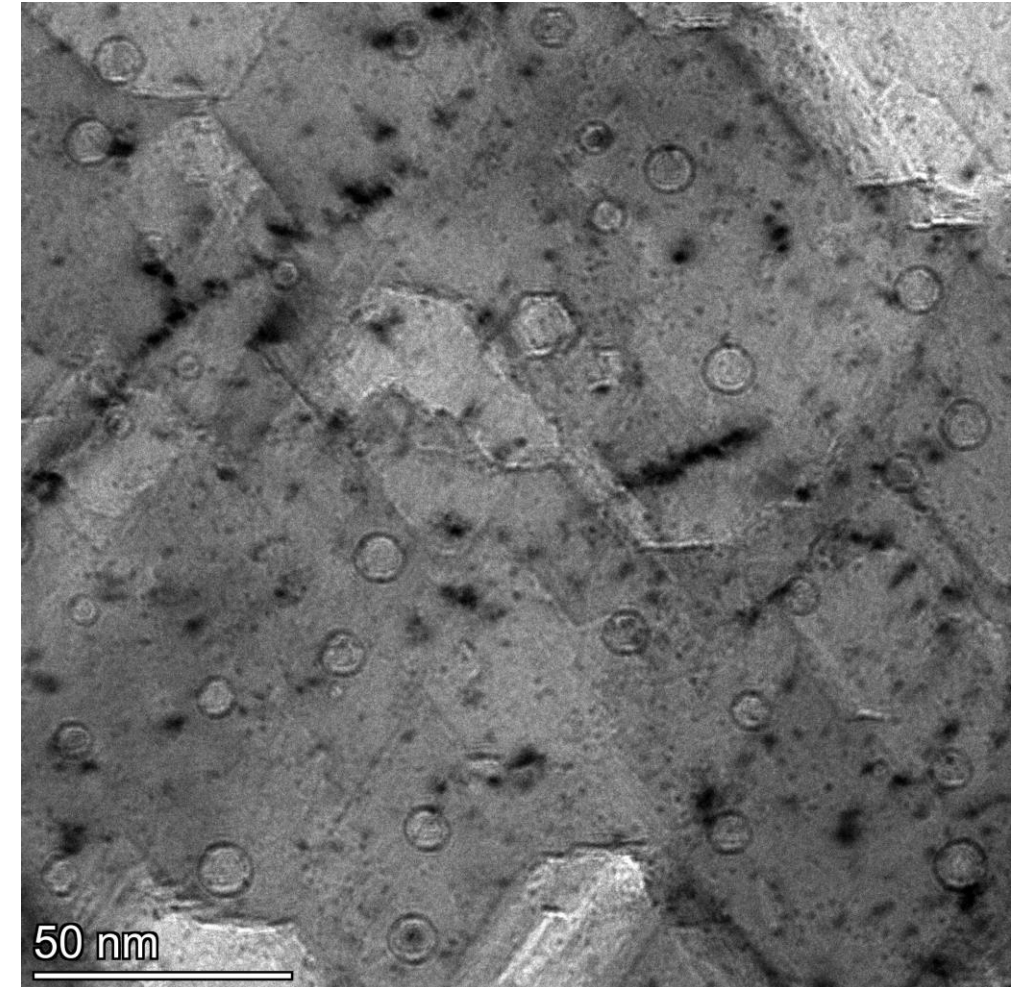
2.3 dpa at 1350 K

## 800 K:

- Similar dependence on dpa as for 290 K
- $D_{\max}$  is 4 times smaller compared with 290 K
- TDS spectra shape similar as for 290 K

## 1350 K:

- No saturation yet
- $D_{\max} = 1.8$  at.% at 2.3 dpa!
- Different TDS spectra compared with 290 and 800 K
- **Change of defect type?**
- **Nanometer-sized voids are visible in TEM**

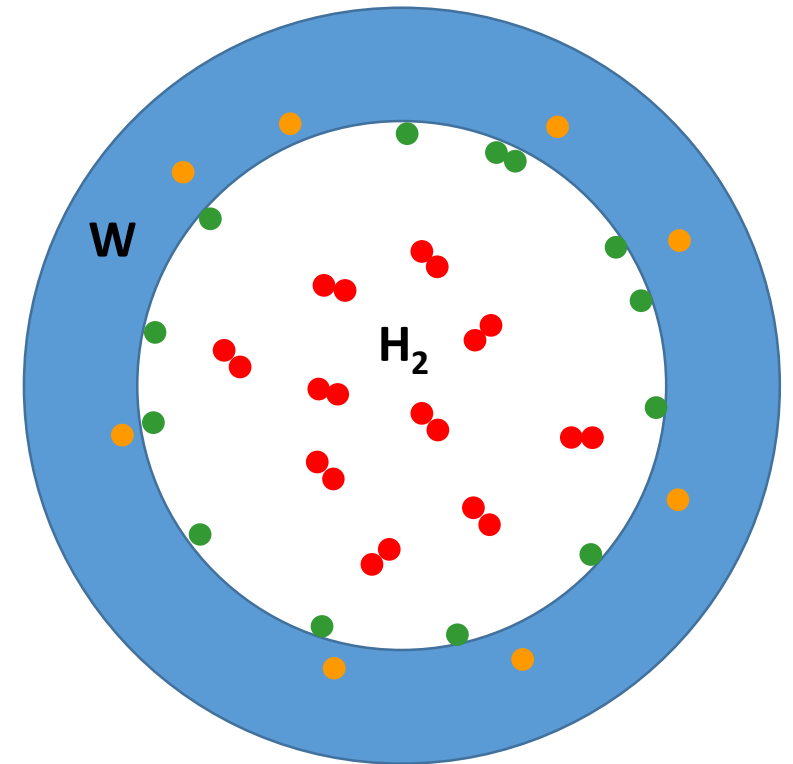


T. Schwarz-Selinger et al., unpublished

# Hydrogen trapping and release from cavities

- Cavities can retain H atoms at the surface and H<sub>2</sub> molecules in the volume
- Different physics compared with 'conventional' traps (vacancies,...)
- Recently developed reaction-diffusion model to describe these phenomena

M. Zibrov, K. Schmid, Nucl. Mater. Energy 30 (2022) 101121  
M. Zibrov, K. Schmid, Nucl. Mater. Energy 32 (2022) 101219



States of H:

1. H<sub>2</sub> gas in cavity volume
2. H atoms adsorbed at cavity surface
3. H atoms in interstitial sites in W

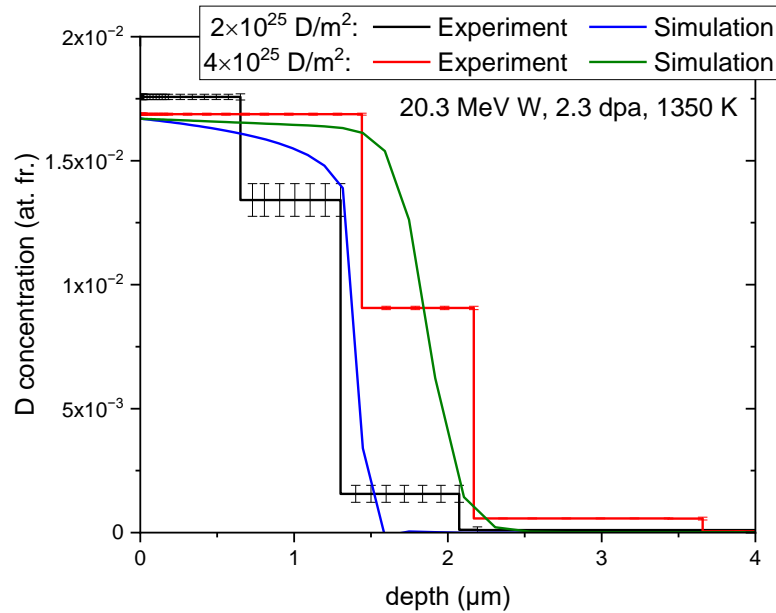




# Simulation results

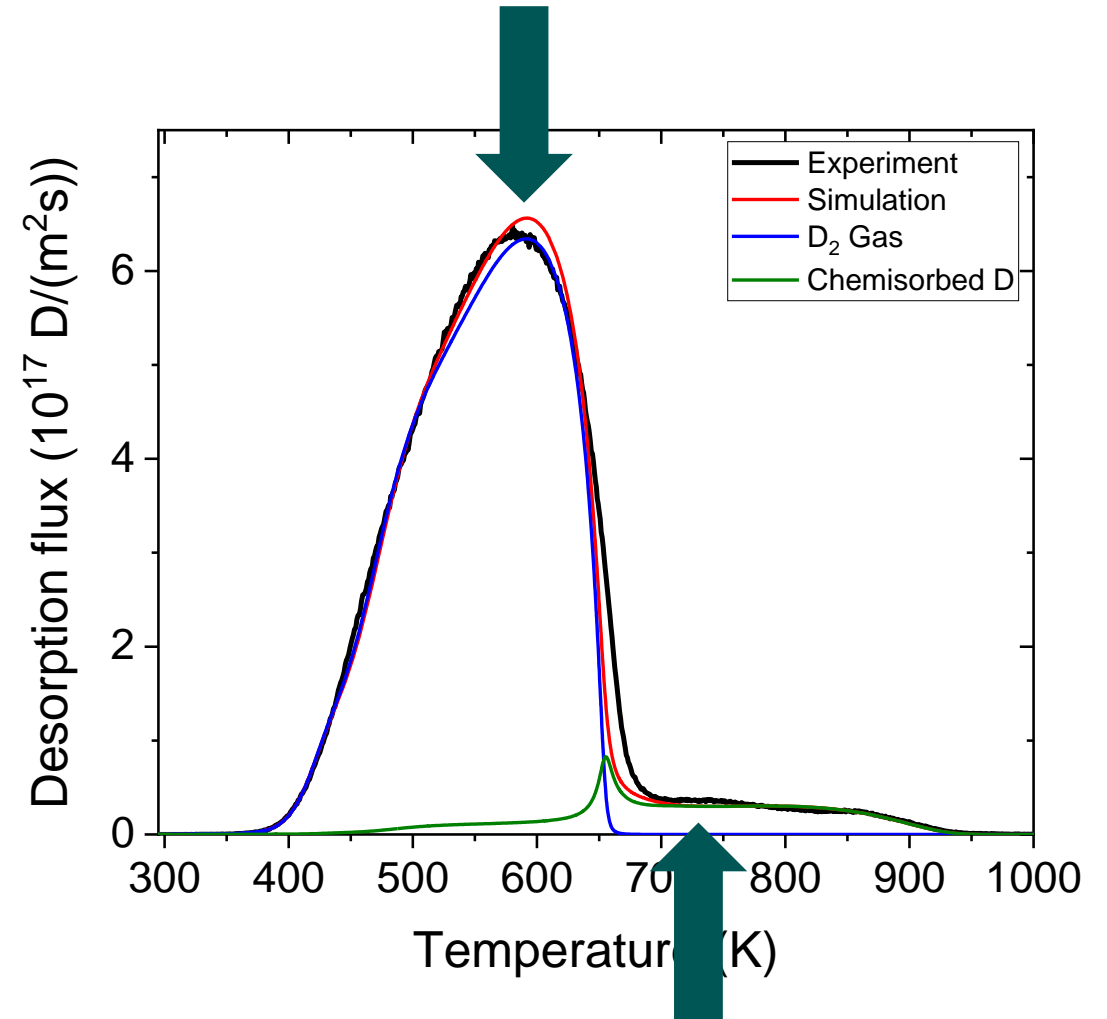
## Model by Zibrov and Schmid

- Can quantitatively describe the experiment
- Reduced solubility of 0.93 eV (Frauenfelder 1.04 eV)
- Very sensitive to bubble size and solute D conc.



- More independent measurements necessary (diff. solute, ...)

D<sub>2</sub> from the cavities

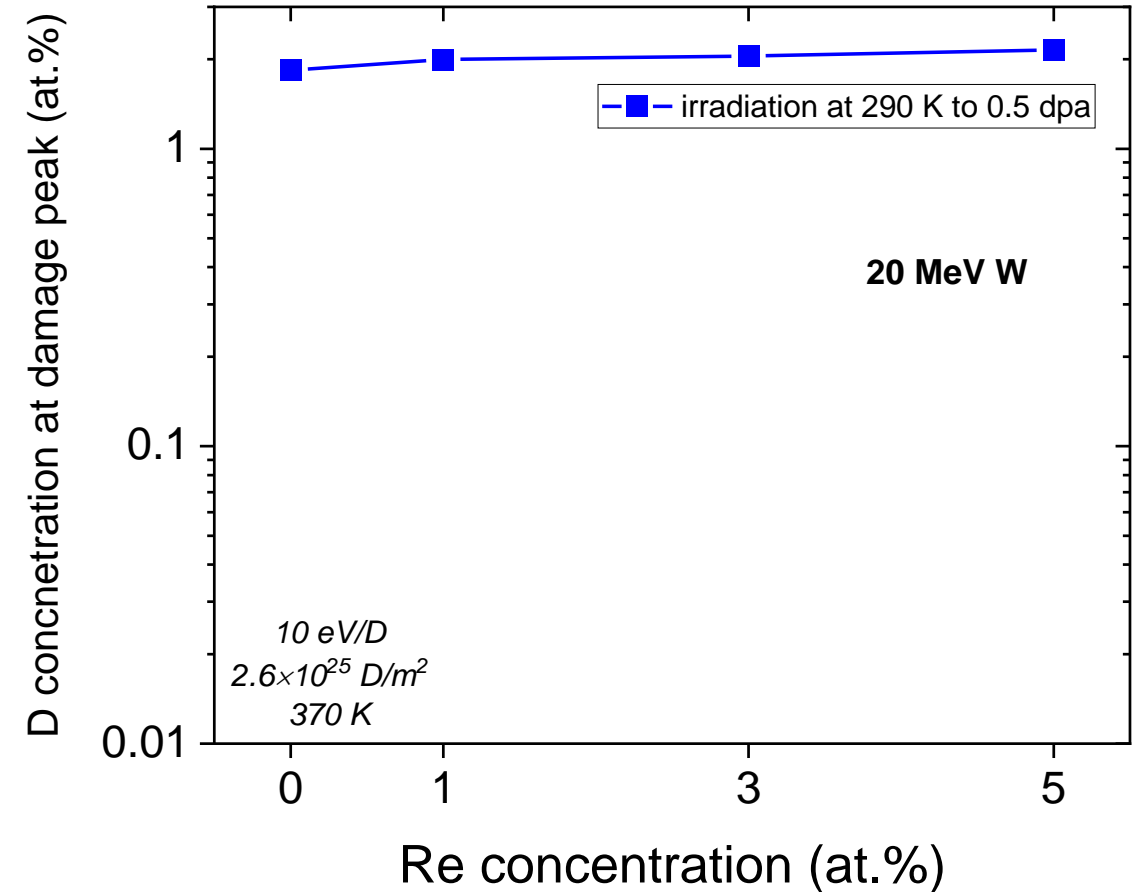


D from cavity surfaces



# Influence of Re on displacement damage in W

- 3.8% Re produced in W after 5 fpy in DEMO
- Synergies between displacement damage and Re production?
- Study W-Re alloys (1–5% Re)
- **290 K**: Little Re effect

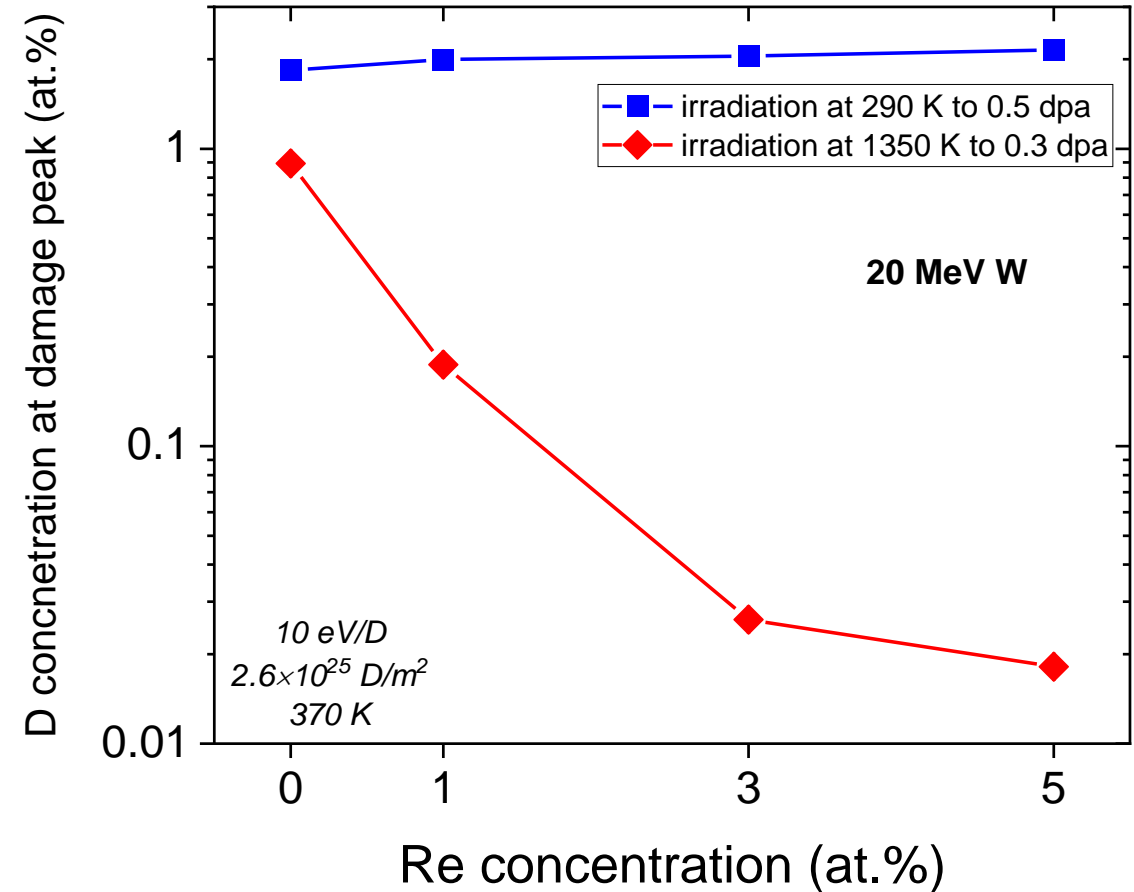


M. Zibrov et al., unpublished



# Influence of Re on displacement damage in W

- 3.8% Re produced in W after 5 fpy in DEMO
- Synergies between displacement damage and Re production?
- Study W-Re alloys (1–5% Re)
- **290 K**: Little Re effect
- **1350 K**: Strong reduction of D concentration with increasing Re concentration

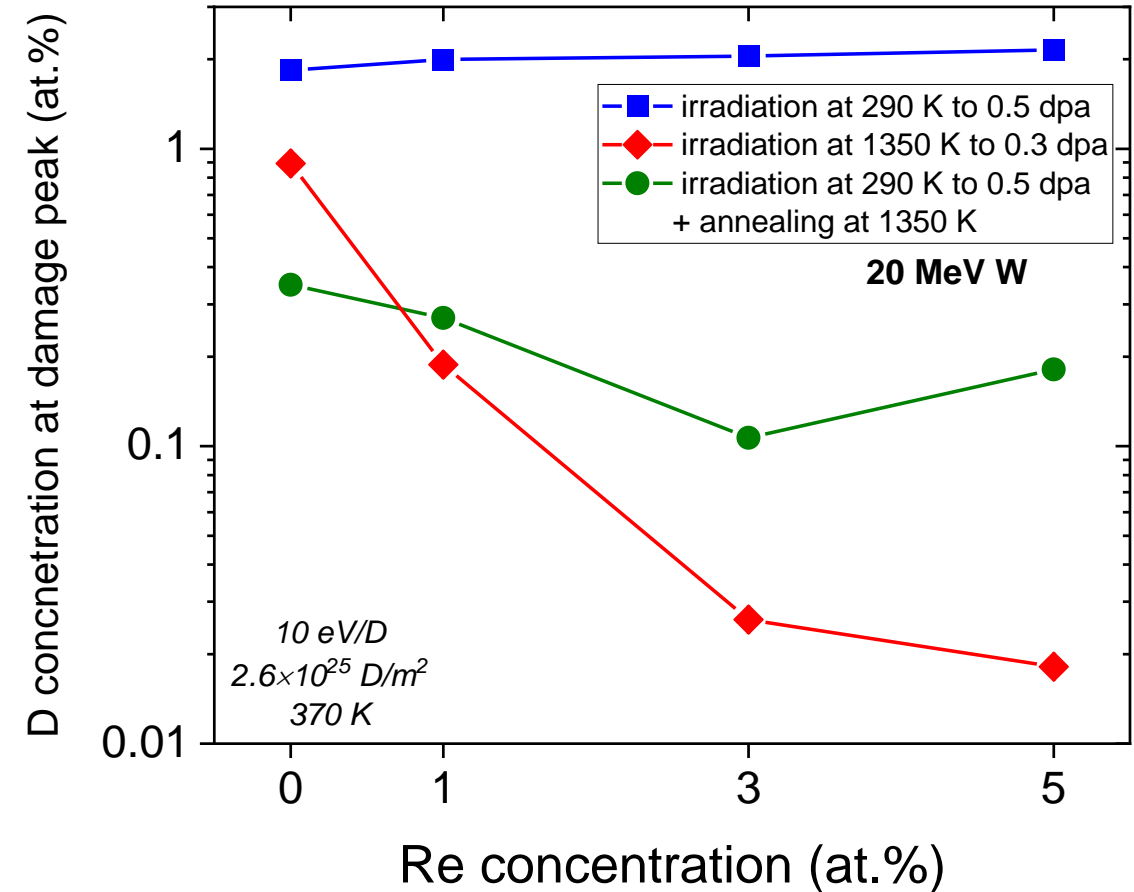


M. Zibrov et al., unpublished



# Influence of Re on displacement damage in W

- 3.8% Re produced in W after 5 fpy in DEMO
- Synergies between displacement damage and Re production?
- Study W-Re alloys (1–5% Re)
- **290 K**: Little Re effect
- **1350 K**: Strong reduction of D concentration with increasing Re concentration
- **290 K + 1350 K annealing**: Milder reduction of D concentration with increasing Re conc.  
⇒ **Irradiation at elevated T is not the same as post-irradiation annealing!**



M. Zibrov et al., unpublished



# Summary

- D concentration
  - saturates for 290 K and 800 K irradiation above 0.1 dpa
  - shows no saturation yet up to 2 dpa for 1350 K irradiation
- Thermal desorption spectra
  - resemble each others for room temperature and 800 K irradiation
  - lack the high temperature peak for the 1350 K irradiation
  - D<sub>2</sub> gas in voids?
- Influence of Re
  - small effect for 290 K irradiation
  - strong reduction of D concentration with increasing Re concentration for irradiation at 1350 K