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

S. Markelj¹, T. Schwarz-Selinger², M. Pečovnik¹, M. Kelemen¹,³

¹Jožef Stefan Institute, Ljubljana, Slovenia
²Max-Planck-Institut für Plasmaphysik (IPP), Garching, Germany
³Jožef Stefan International Postgraduate School, Jamova cesta 39, 1000 Ljubljana, Slovenia

This work has been carried out within the framework of the EUROPefusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.
Tungsten - plasma facing material

Fusion device scenario

D/T plasma exposure + neutron irradiation

D,T

n - 14 MeV
Neutron bombardment = Displacement damage creation

Damage creation at RT + damage annealing

Damage creation at elevated temperatures

Vacancy

Self-Interstitials

Dislocation

Vacancy cluster
Tungsten – plasma facing material

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

Neutron bombardment
= Displacement damage creation

Damage creation at RT + damage annealing

Damage creation at elevated temperatures

Fuel transport:
diffusion trapping de-trapping

Fuel retention

D,T

n - 14 MeV

Implantation Reflection Adsorption Recombination

Diffusion Desorption Trapping

Vacancy
Dislocation
Vacancy cluster Self-Interstitials Interstitials
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

Damage creation at RT + damage annealing

Damage creation at elevated temperatures

Fuel transport: diffusion trapping de-trapping

Fuel retention

S. Markelj et al. | MoD PMI 2019, Japan | Page 5
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
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

Ion damaging
- Few µm

neutron damaging
- Few cm

SRIM calculation of ion trajectory

W self-damaging

20 MeV W in W

20 µm

1 µm
Displacement damage creation by MeV W ion irradiation

- W self-damaging
- W ion irradiation by MeV W ions
  - Creation of displacement damage

Displacement damage creation
MeV W ion irradiation

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

D atom exposure @ 600 K

10.8/20 MeV W irradiated

 bulk W
Simultaneous W/D exposure

Simultaneous W/D exposure:  
W ion irradiation  
D exposure  
@ different high temperatures

≈ 2µm
recrystallized

bulk W
Simultaneous W/D-D exposure:

- **W** ion irradiation @ different high temperatures
- **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 $3.7 \times 10^{23} \text{ D/m}^2$

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

Atom flux = $5.4 \times 10^{18} \text{ D/m}^2\text{s}$
$\Gamma_D = 8 \times 10^{22} \text{ D/m}^2$

W fluence = $1.4 \times 10^{18} \text{ W/m}^2$
Dose $\rightarrow 0.47 \text{ dpa}_{KP}$
Displ. Rate $= 3 \times 10^{-5} \text{ dpa/s}$
Effect of D presence – atom exposure
Comparison of D concentration

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

Comparison to different damaging procedures

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

![Graph showing the effect of temperature on D concentration](image)
Effect of D presence – atom exposure
Comparison of D concentration

- 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:
- E. Hodille et al. Nucl. Fusion 59 (2019) 016011
Experiment with ions– 300 eV/D

- Simultaneous/sequential W/D, W-D ion loading
- Defect population - exposure D ions @ 450 K – fluence $2.7 \times 10^{23} \text{ D/m}^2$

Ion energy 300 eV/D
Ion flux=1.3x10$^{18}$ D/m$^2$s
$\Gamma_D=1.9 \times 10^{22} \text{ D/m}^2$

W fluence = 1.0x10$^{18}$ W/m$^2$
Dose $\rightarrow$ 0.35 dpa$_{KP}$
Displ. Rate = 2.4$\times$10$^{-5}$ dpa/s

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

- M. Pecovnik et al. submitted to Nucl. Fusion
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 @ 450 K
D ion exposure

4h simultaneous W/D
W ions – flux $9.73 \times 10^{13}$ W/m$^2$s – 0.34 dpa
D ions - Ion flux=1.4x10$^{18}$ D/m$^2$s
$\Gamma_D=2.0\times 10^{22}$ D/m$^2$
Simultaneous W/D exposure @ 450 K
D depth profile
Simultaneous W/D-D exposure @ 450 K

Simultaneous W/D-D exposure:
- **W ion irradiation** at 450 K
- **D ion exposure**
  - + **D ion exposure** at 450 K – to populate created traps

4h simultaneous W/D
- W ions – flux $9.73 \times 10^{13}$ W/m$^2$s – 0.34 dpa
- D ions - Ion flux=$1.4\times10^{18}$ D/m$^2$s.
- D fluence=$2.0\times10^{22}$ D/m$^2$
  - + 41h D ion exposure - D fluence $2.1\times10^{23}$ D/m$^2$
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 $9.73 \times 10^{13} \text{ W/m}^2\text{s} – 0.34 \text{ dpa}$

+ 39h D ion exposure - D fluence $2.0 \times 10^{23} \text{ D/m}^2$
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
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

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

300 eV/D ion exposure at 450K

![Graph showing the relationship between irradiation temperature (T_exp) and maximum D concentration (at. %). The graph illustrates a decrease in D concentration with increasing temperature, indicating less damage at higher temperatures.](image-url)


- **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
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

Fusion device scenario neutron irradiation during D/T plasma exposure

Two possible effects

- **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
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:

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

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 $\alpha_i$.

$\Gamma$ ... W ion flux (W m$^{-2}$s$^{-1}$)
$\eta$ ... Creation probability (m$^{-1}$)
$\theta(x)$ ... SRIM dam. distribution (1)
n$_{i,\text{max}}$ ... Saturation density (1 (at. fr.))
Stabilization by trapped D

TDS

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

D depth profiles

Comparison of sequential vs. simultaneous @450 K

Normalized D desorption [f]

Temperature [K]

D fraction [at. fr.]

Depth [μm]
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
- M. Pečovnik et al. under review Nucl. Fusion

References atoms:
- E. Hodille et al. Nucl. Fusion 59 (2019) 016011
D mobile concentration comparison