Comparison of deuterium trapping in ion- and neutron- damaged tungsten

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Acknowledgement

HGF grant to perform experiments at IPP (Garching)

K. Sugiyama for NRA measurements

J. Doerner, M. Fußeder and G. Matern
for technical assistance

Accelerator & n-irradiation

Simulation of n damage with charged particle irradiation

- ***Advantage***
- **Ion beams produce displacement damage at much faster rate than neutrons (Higher damage rate 10^{-4}–10^{-2} dpa/s accelerator vs 10^{-6}–10^{-10} dpa/s reactor)**
- **Good control of experimental parameters**
- **Irradiated specimens are not radioactive**
- **Only one possible choice in the absence of high flux neutron irradiation facility**

- ***Disadvantage***
- **Difference in recoil spectra and damage morphology**
- **Charged particle damage is produced very inhomogeneously and its maximum is situated at a certain depth in the irradiated sample. While neutrons will create damage distributed over all material thickness**
- **Stress induced by irradiation – surface proximity**

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Self-ions as surrogate for n irradiation

Accelerator & n-irradiation

Simulation of n damage with charged particle irradiation

How accurate the neutron-produced damage in W

can be simulated by irradiation with self-ions

Radiation damage

Self-ion irradiation was done at IPP

20 MeV W^{6+}, RT

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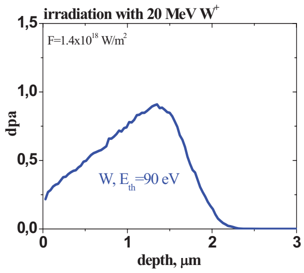
- Damaged depth ~2.5 µm
- Beam sweep unit for homogeneous irradiation of larger areas (20 mm)
- Well defined fluence control by 4 corner Farraday cups



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Neutron irradiation was done in HFIR at Oak Ridge National Laboratory by big scientific group [Hatano et al., NF, 2013]

Irradiation with mixture of

fast neutrons >0.1 MeV
with flux of 8.9×10^{18} $m^{-2}s^{-1}$ and

thermal neutrons with flux of
2.5×10^{19} $m^{-2}s^{-1}$

Exposure of damaged samples to D plasma

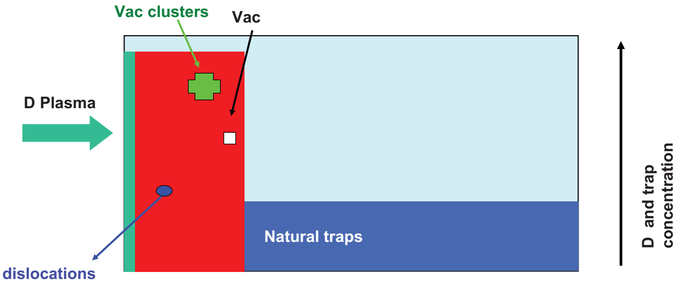
Exposure to low-energy D plasma:

W pre-damaged with self-ions:
5 – 20 eV with ion flux of 10^{20} D/m^{2}s

W pre-damaged with neutrons:
100 eV per D with ion flux of ~$6x10^{21}$ D/m^{2}s

Radiation damage produced by self-ions

Radiation damage up to ~ 1 dpa, RT



Radiation damage produced by neutrons

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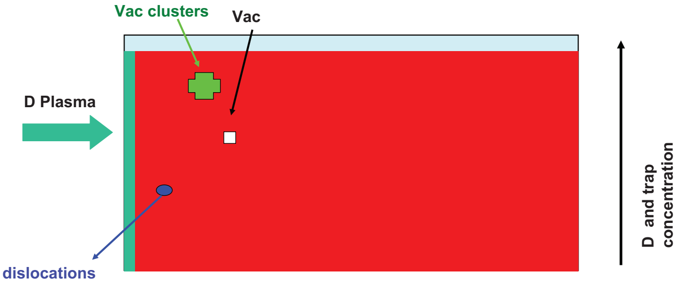

Deuterium decoration of radiation damage

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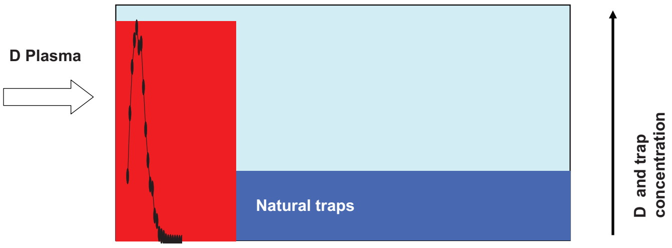
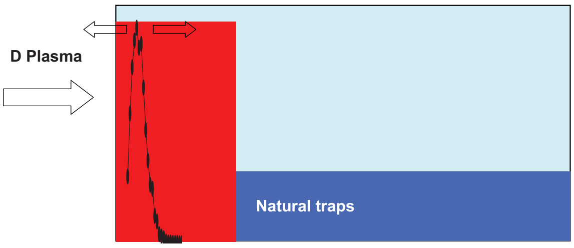


Deuterium decoration of radiation damage

Radiation damage up to ~ 1 dpa, RT

$x=2(1-r)I_0tR_p/W_t(T)$

x(time)=2*(*fluence*ion projected range)/(density of traps)*



O.V. Ogorodnikova and K. Sugyama, JNM, 2013

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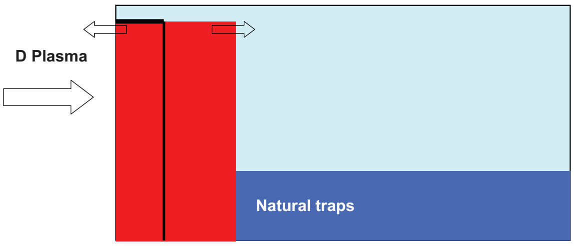

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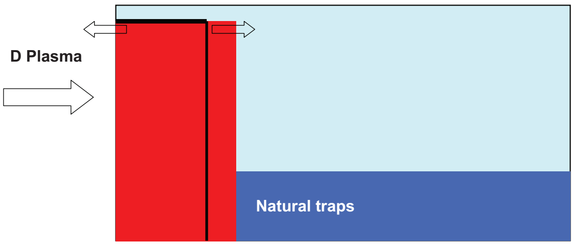

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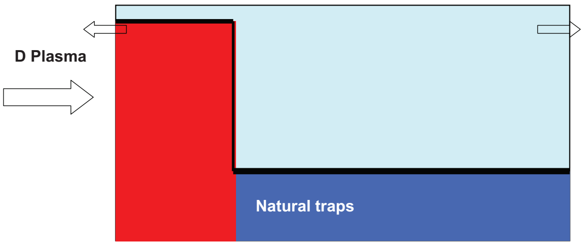

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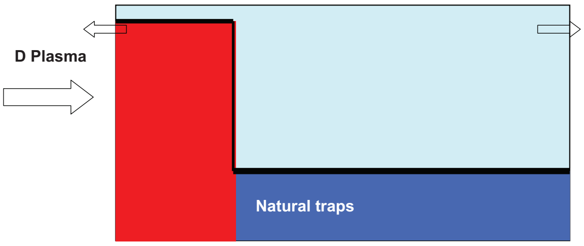


Depth profile was measured by NRA up to 6 microns

Deuterium decoration of radiation damage

D plasma was exposure at 470 K to decorate defects with low and high binding energy for D (dislocations, grain boundaries, vacancy, vacancy clusters)

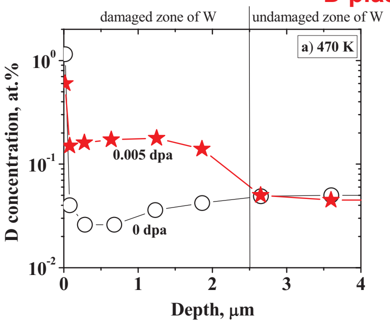
D Plasma

D plasma was exposure at 700-773 K to decorate defects with high binding energy for D (vacancy clusters)

Deuterium decoration of radiation damage

20 MeV W $^{6+}$

D plasma exposure at 470 K



D is trapped at radiation-induced defects produced by self-ions up to ~ 3 μm.

Deuterium decoration of radiation damage

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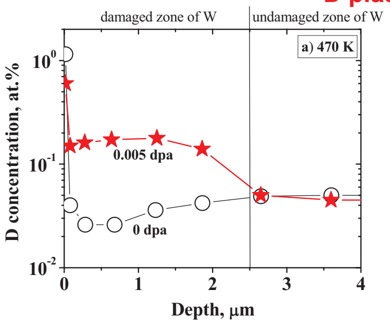

Early damage formation with self-ion irradiation already at 0.005 dpa

in agreement with TEM observation [X. Yi , M.L. Jenkins, M. Briceno, S.G. Roberts, Z. Zhou, M.A. Kirk, Philosophical Magazine, 2013]

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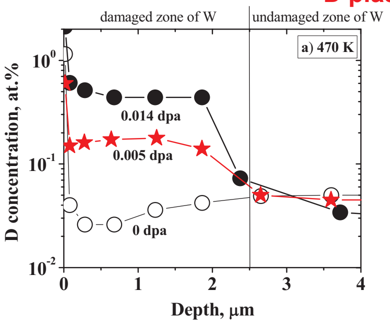

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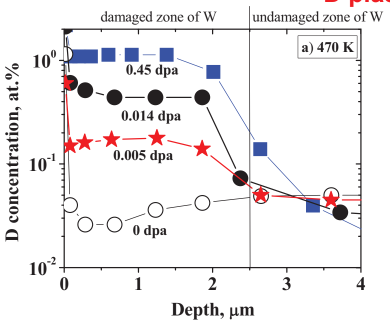

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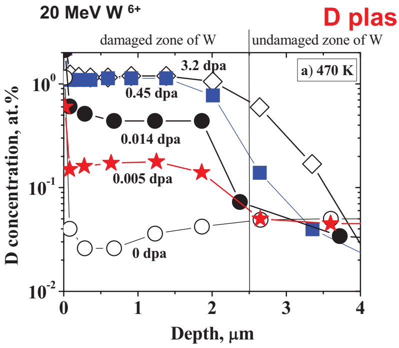

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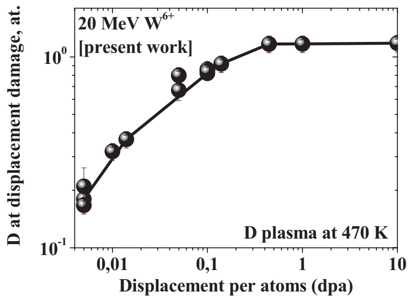

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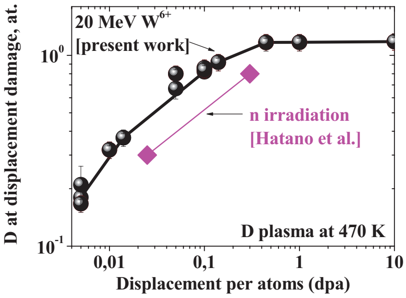
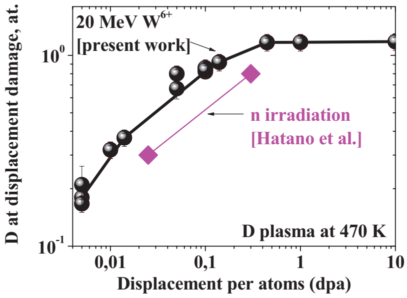


K_{exp}=0.65

Deuterium decoration of radiation damage

D plasma at 470 K

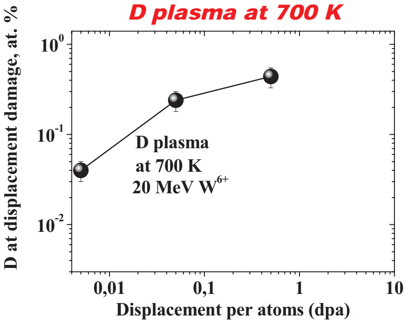


K_{exp}=0.65

This means that being irradiated up to the same dose (in dpa) neutron-irradiated W retains only ~65% of the deuterium that retains in self-ion irradiated W

Deuterium decoration of radiation damage

D plasma at 700 K

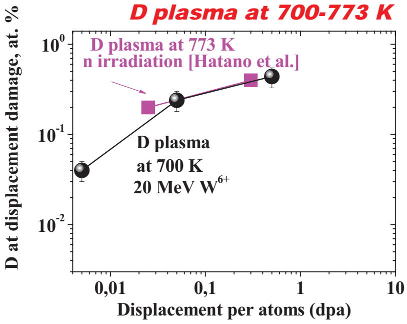


D occupied only vacancy clusters

D de-populated from defects with low binding energy (dislocations, grain boundaries)

Deuterium decoration of radiation damage

D plasma at 700-773 K



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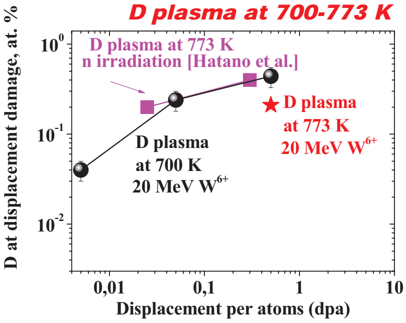


K_{exp}=0.73

Modelling

Calculations include all stages of experimental procedure:

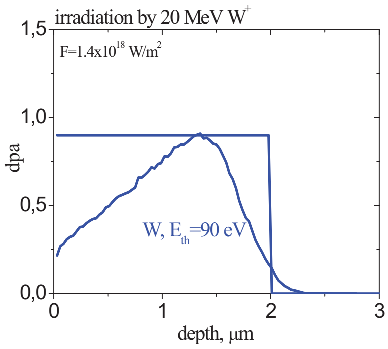
(i) implantation of deuterium into tungsten from plasma,

(ii) cool down stage,

(iii) time delay between the end of implantation and the start of depth profile measurements

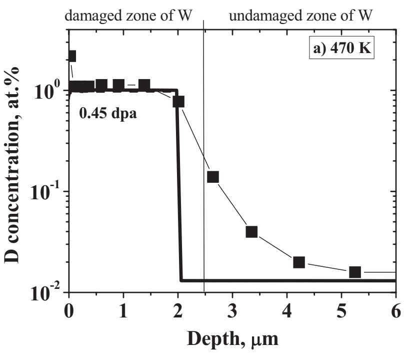
O.V. Ogorodnikova et al., JNM, 1999

Deuterium decoration of radiation damage



Deuterium decoration of radiation damage 470 K

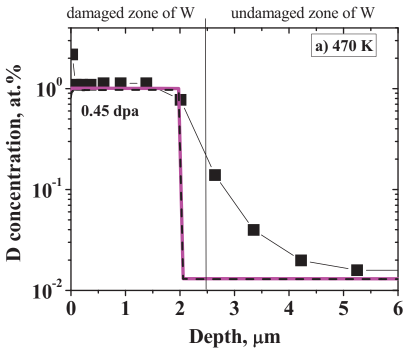
Ion flux: $I_0=10^{20}$ D/m^{2}s



Similar implantation profile and post-mortem D depth profile

Deuterium decoration of radiation damage 470 K

Ion flux: I_0=6x10^{21} D/m^{2}s

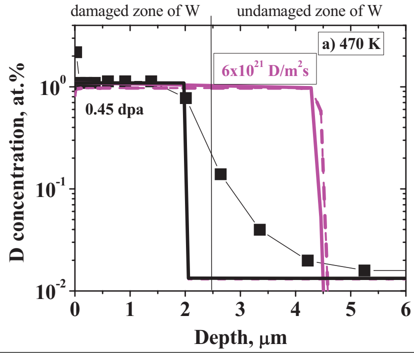


No effect of ion flux

Similar implantation profile and post-mortem D depth profile

Deuterium decoration of radiation damage 470 K

radiation-induced defects produced by neutrons with Ksim=1



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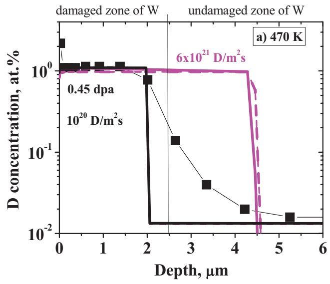
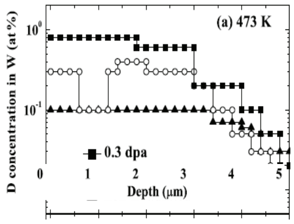
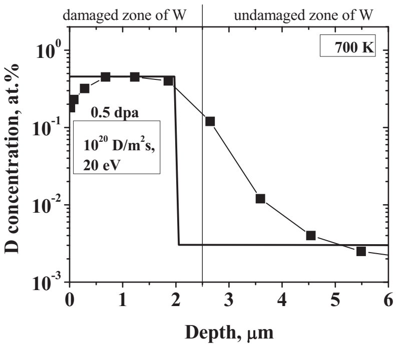


neutrons in HFIR (E>0.1 MeV) [Hatano et. al, NF, 2013]



Deuterium decoration of radiation damage 700 K

Ion flux: I_0=10^{20} D/m^{2}s



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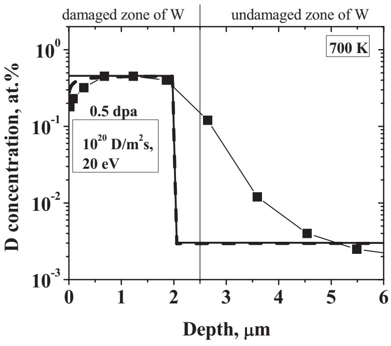

Similar implantation profile and post-mortem D depth profile

Deuterium decoration of radiation damage 700 K

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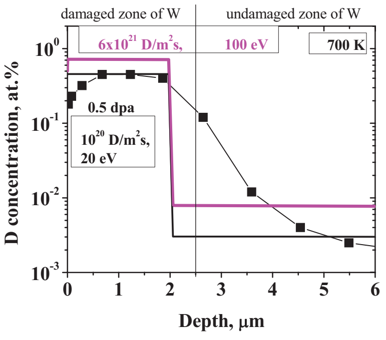

An increase of the trapped D under implantation with increasing of the ion flux

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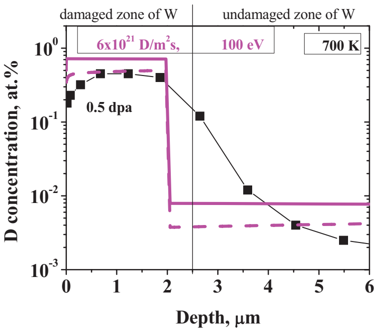
Deuterium decoration of radiation damage 700 K

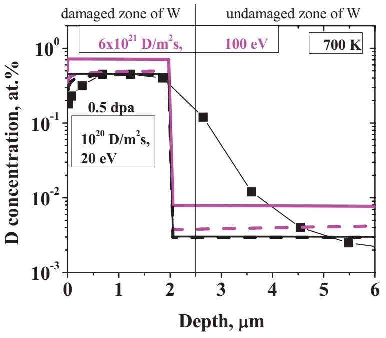
Ion flux: I_0=6x10^{21} D/m^{2}s



Lower post-mortem D depth profile compared to dynamic depth profile.

Release of weakly bonded D during slow cooling

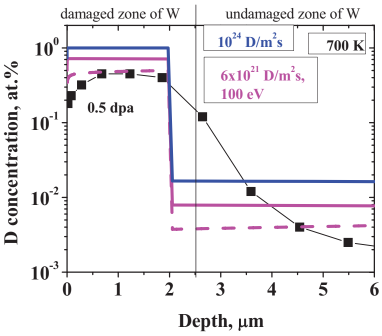
Deuterium decoration of radiation damage 700 K



Similar post-mortem D depth profile for both ion fluxes after cool down

Deuterium decoration of radiation damage 700 K

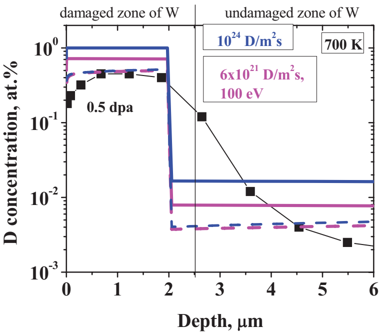
Ion flux: $I_0=10^{24}$ D/m²s



Dynamic depth profile is higher for high ion flux.

Deuterium decoration of radiation damage 700 K

Ion flux: $I_0=10^{24}$ D/m²s



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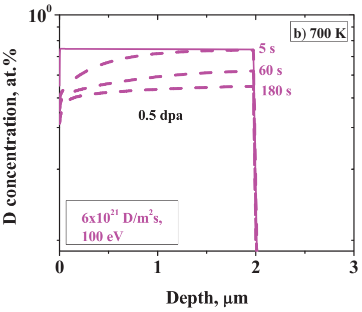
Release of weakly bonded D during slow cooling

Influence of t_{after}

20 MeV W $^{6+}$

Ion flux: $I_0=6x10^{21}$ D/m²s



Time of keeping of the sample at irradiation temperature after the plasma was switched off

Release of weakly bonded D during cooling

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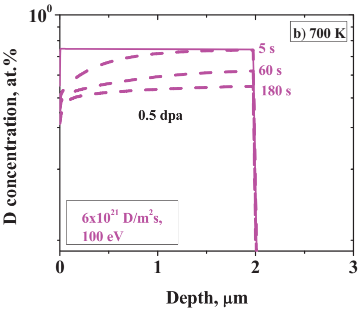

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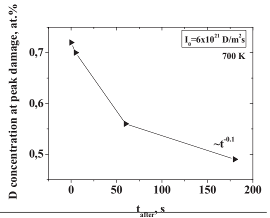

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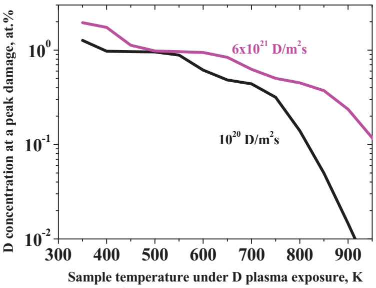


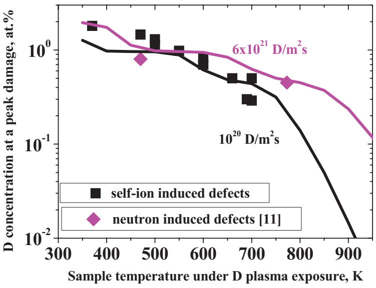
An increase of the ion flux increases the trapped D:

Trapped D = f (ion flux)

$$Y=\sum_{k=1}^{m}\sum_{j=1}^{f_k} f_k W_{tk}/(1+(D_0\ z\rho_{me}\exp(-E_{tk}^{j}/kT))/((1-r_{ion})I_0 R_p)).$$

O.V. Ogorodnikova et al., JNM, 1999

Deuterium decoration of radiation damage



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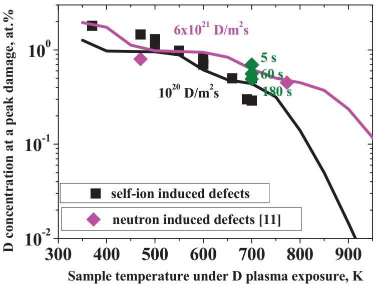
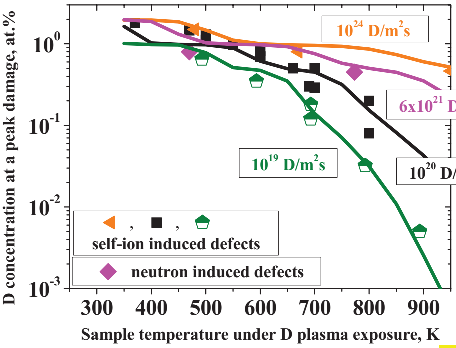


Effect of enhanced D trapping in W at high flux



10^{24} D/m²s: Wright et al, NF, 2010

6x10^{21} D/m²s: Hatano et al., NF, 2013

10^{20} D/m²s: O.V. Ogorodnikova & K.Sugyama., JNM, 2013

10^{19} D/m²s: O.V. Ogorodnikova and S. Markelj, in preparation

O.V. Ogorodnikova, JAP, 2015

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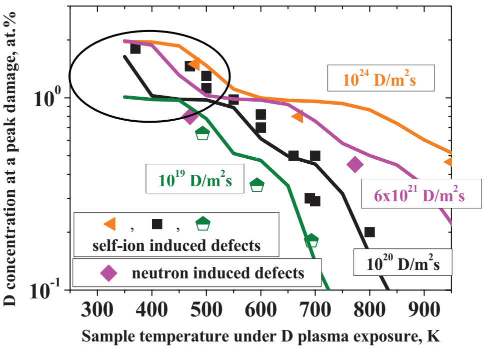

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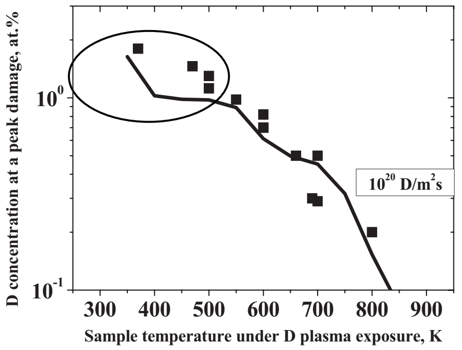

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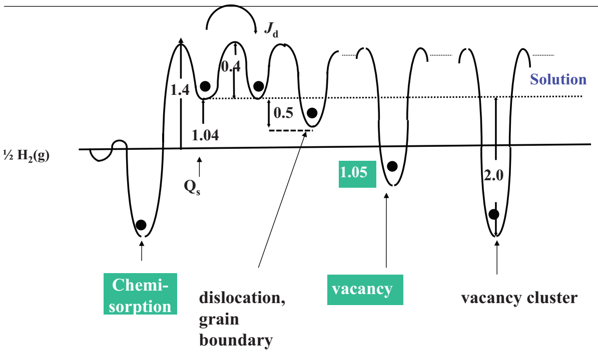

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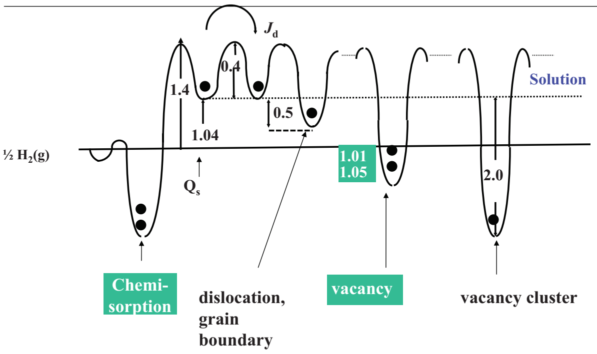

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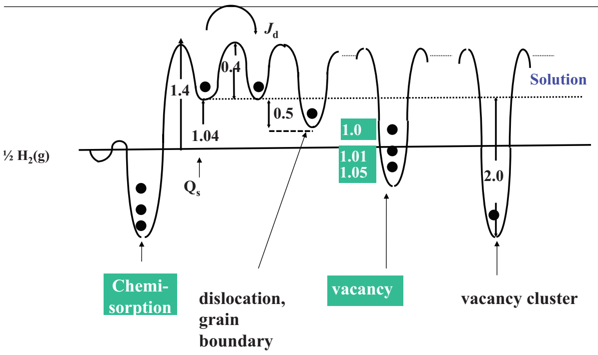

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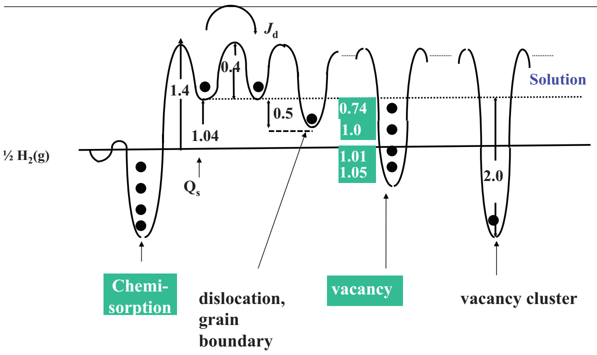
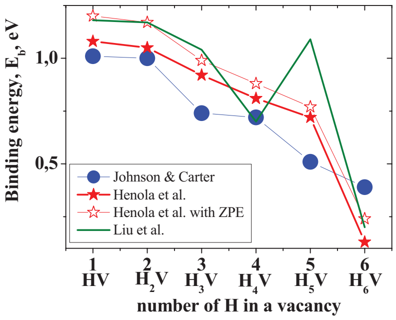
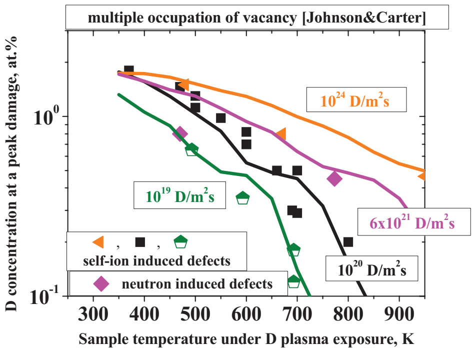


Multiple occupation of a vacancy by DFT



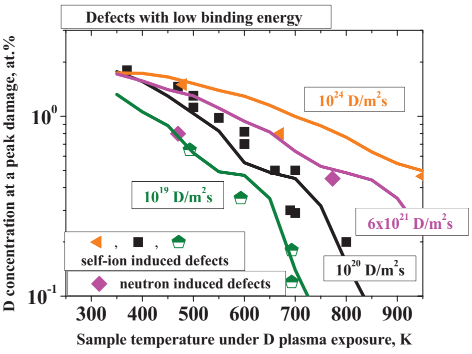
Multiple occupation of a vacancy



Multiple occupation of a vacancy improves an agreement between model and experiment at low temperature range

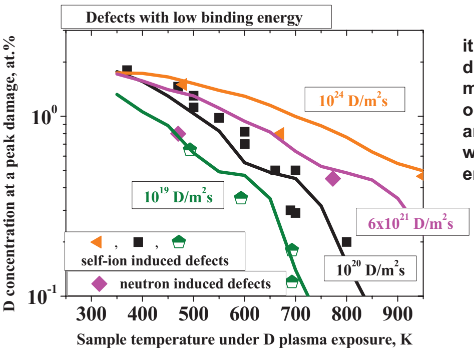
It is possible to validate DFT models: Only model of Johnson&Carter improves agreement with experimental data

The range of defects with low binding energy



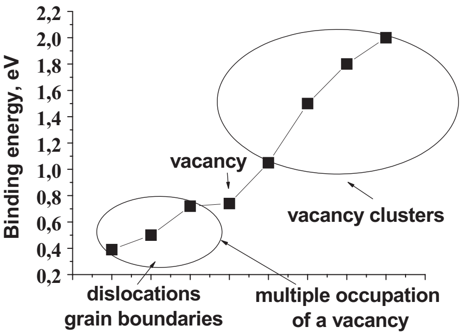
Range of defects with low binding energy for D improves an agreement between model and experiment at low temperature range

The range of defects with low binding energy

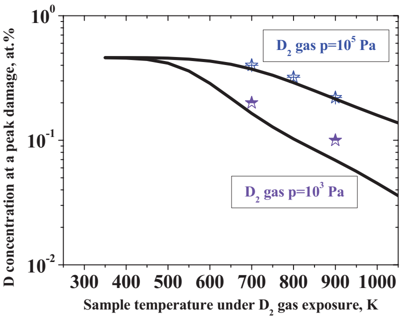


it is impossible to distinguish between mechanisms of multiple occupation of a vacancy and range of defects with closely binding energy and trap density

Defects in W

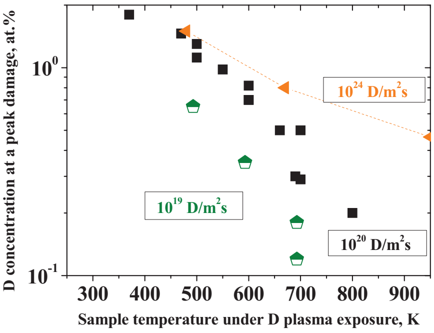


Validation of model against exposure to D_2 gas

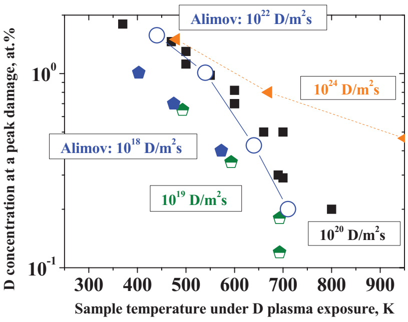


No free parameters!

Effect of enhanced D trapping in W at high flux



Effect of enhanced D trapping in W at high flux



Alimov et al. data are not in an agreement with present database. Why?..

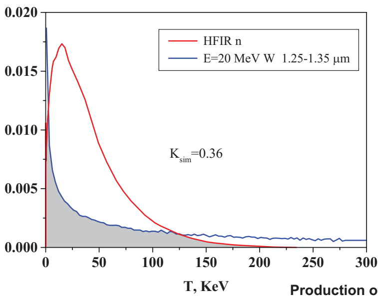
Theoretical value of coefficient of similarity

O. V. Ogorodnikova[1] and V. Gann[2]

[1]*National Research Nuclear University MEPhI, Moscow, Russia*
[2]*National Science Centre “Kharkov Institute of Physics and Technology”, Kharkov, Ukraine*

Theoretical value of coefficient of similarity

K_{sim}=0.36



Classical damage energy function as a function of PKA

a fraction of common area under two curves $W_n'(T)$ and $W_i'(T)$

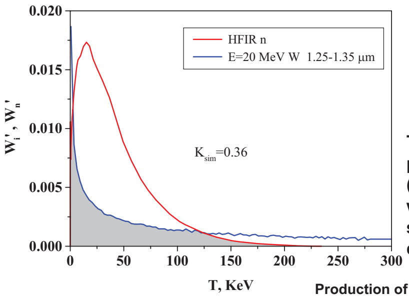
Classical model

The value K_{sim} is averaged part of displaced atoms (over the all PKA spectrum), which were produced in the similar conditions under two different types of irradiation.

Production of primary knock-on atom (PKA) spectrum by cascade function is called in literature as damage energy spectrum.

O.V. Ogorodnikova and V. Gann, JNM, 2015

Theoretical value of coefficient of similarity



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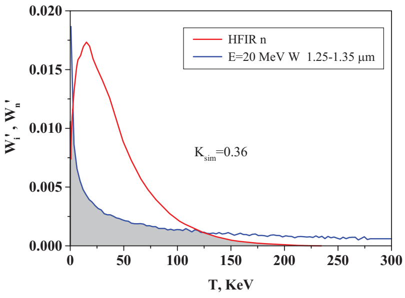

Classical damage energy function as a function of PKA

K_{sim}=0.36

K_{exp}=0.65

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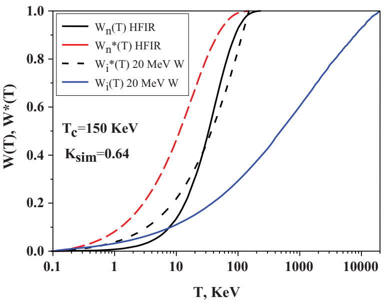
Theoretical value of coefficient of similarity



Energy-reduced damage function W*(T) as a function of PKA

K_{sim}=0.64

for T_c=150 keV

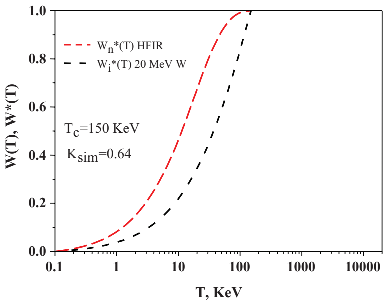
Model of reduced PKA spectrum

All cascades with an energy higher than T_c split into identical sub-cascades

T_c is cascade break-up threshold energy

PKAs with energy more than T_c=150 keV as external fast ions

Theoretical value of coefficient of similarity



Energy-reduced damage function W*(T) as a function of PKA

K_{sim}=0.64

for T_c=150 keV

K_{exp}=0.65

Splitting of high-energy part of cascades might take place in W that results in a reduction of the effective PKA spectrum and a change of types and density of post-radiation defects.

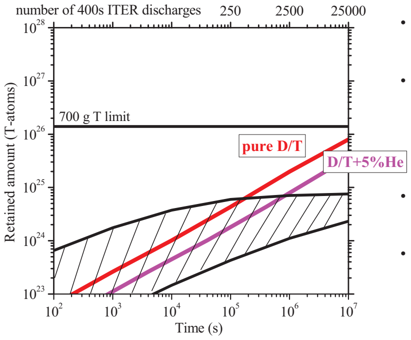
Summary

- **Theoretical value of coefficient of similarity between neutrons and self-ion irradiation of W was derived**
- **Experimental value of coefficient of similarity was found by comparison of the deuterium concentration at radiation-induced defects produced with MeV self-ion irradiation and neutrons irradiation in HFIR and compared with theoretical value**
- **Two models, (i) the classical damage energy spectra and (ii) fragmentation cascades into sub-cascade, were verified by comparison with experimental data. It was shown that the model assuming that all cascades with an energy higher than *Tc*=150 keV split into identical sub-cascades is in an agreement with experimental value. Classical model results in underestimation of coefficient of similarity**
- **Effects of ion flux and cooling rate on measurements of deuterium post-mortem depth profile were modelling and their influence on the coefficient of similarity was estimated**

Main conclusion

- **Self-ion irradiation provides a convenient and reliable method of simulating damage from low neutron doses without any problem of long irradiation time and significant activation of the specimens.**
- **A difference between n- and self-ion irradiations can increase at high irradiation fluence due to a production of sufficient amount of helium (He) and transmutation products under n-irradiation in contrast to ion irradiation.**

Neutron damage: prediction for ITER



- **n-irradiation damage enhances the T inventory**
- **He seeding in D/T plasma decreases hydrogen isotopes diffusion into the bulk but does not change the D trapping in radiation damages**
- **The T retention does not reach a limit during the ITER lifetime**
- **The T retention could be a concern for the DEMO**

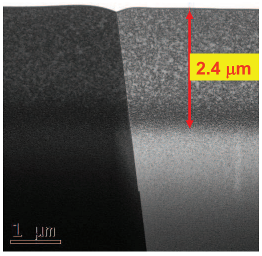
O.V. Ogorodnikova et al., JNM, 2011

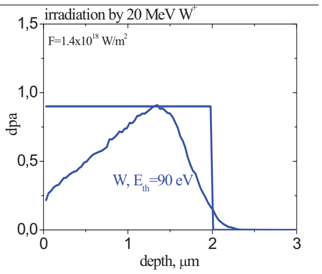
Deuterium decoration of radiation damage 700 K

Important parameters leading to uncertainties in evaluation of *Kexp* are ion flux and cooling rate.

Measurements of the D retention after ion- and neutron irradiation at identical plasma conditions are necessary to draw a final conclusion

Radiation damage



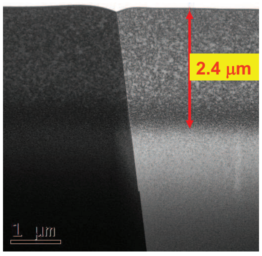


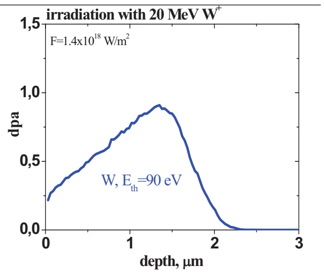
TEM for W (L. Ciupinski et al.):
Damage up to 2.4 μm

Flat depth profile was created by implantation with different energies

20 MeV W^{6+} $F=1.4x10^{18}$ W^{6+}/m^2 (0.89 dpa)
8 MeV $F=3.06x10^{17}$ W^{6+}/m^2
4 MeV $F=1.97x10^{17}$ W^{6+}/m^2
2 MeV $F=1.38x10^{17}$ W^{6+}/m^2

Radiation damage





TEM for W (L. Ciupinski et al.):
Damage up to 2.4 μm

Calculation by SRIM:
Damage up to 2.4 μm

Calculation of damage profile by SRIM is in a good agreement with TEM observation