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Temperature dependence of deuterium retention at displacement damage in tungsten

PB-076

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Introduction

Displacement damage from fusion neutrons increases retention of deuterium (D) and tritium (T) in tungsten exposed to DT plasma. The enhanced retention strongly depends on temperature due to:

a) DT diffusion and kinetics of permeation to the damage,

b) finite binding energy to the damage, and

c) annealing of damage.

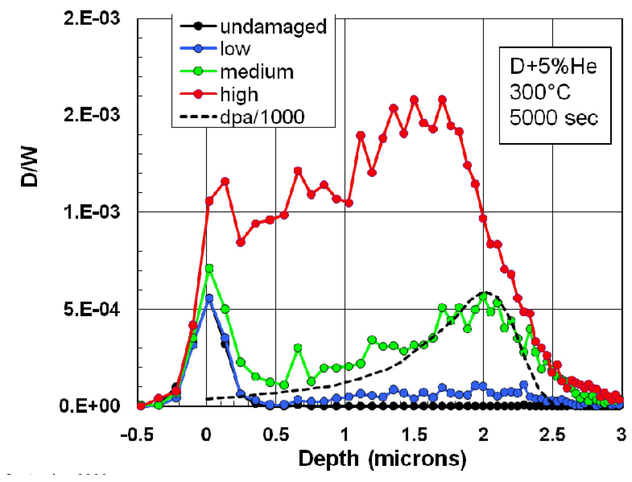
Here we examine how these factors influence DT retention at displacement damage in tungsten.

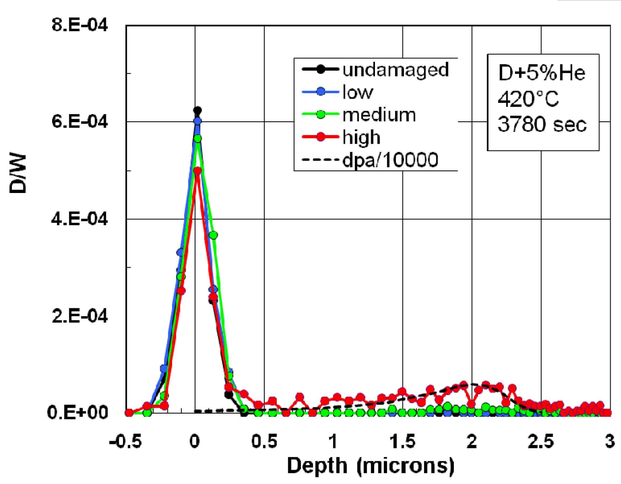
Experiment

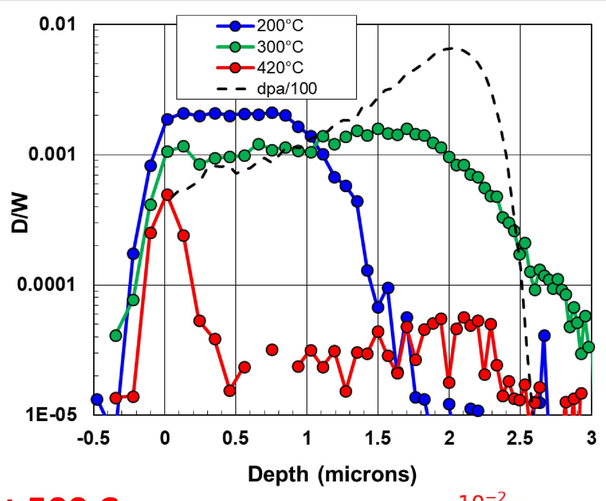
1. Simulate neutron damage using 12 MeV Si ion irradiation.
   Produces ~ 7500 displacements per ion, up to 0.6 dpa at 2 µm.
2. Simulate exposure to divertor plasma
   using D plasma in PISCES A, by R.P. Doerner at UCSD.
   low energy (~100eV), high flux ($2x10^{18}$ D/cm^{2}s)
   & fluence (10^{22} D/cm^2), at T = 40 to 500°C.
3. Measure resulting D concentration vs depth to 3µm
   by D(^{3}He,p)α NRA.

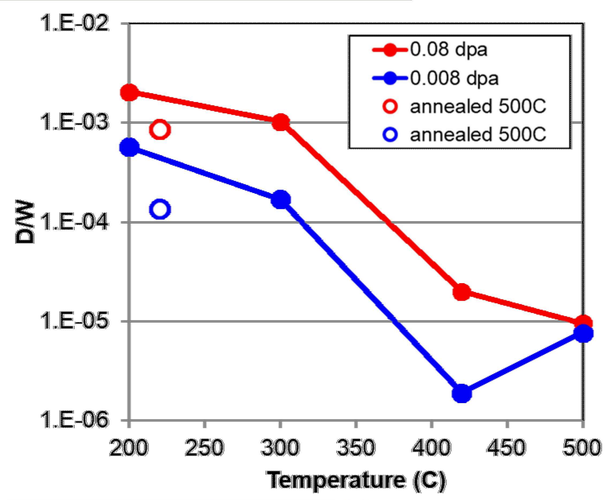
Damage & D + 5% He plasma, T=200, 300, 400, 500°C

Damage & D + 5% He plasma at 200°C after 500°C anneal.





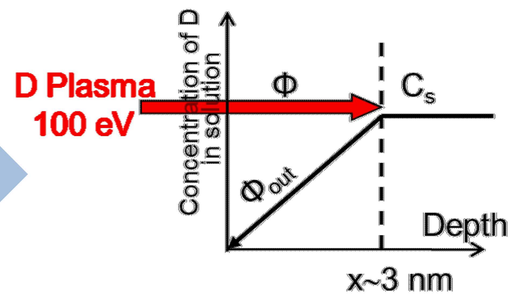


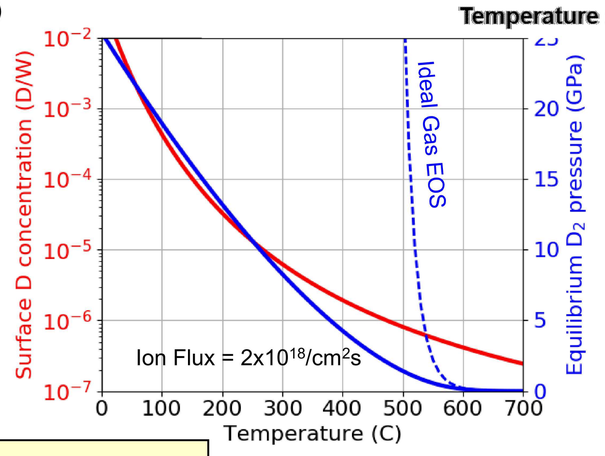


100x decrease between 300 & 400C but only 2x reduction after annealing at 500 C.
Lower D retention at T>400C is mostly due to weak binding, not defect annealing.

Model for D retention at displacement damage

1. Implantation from plasma with diffusion-limited release gives near-surface concentration: smaller at higher T.
   $$C_s = \frac{\phi_D \, x}{D \, N_W}$$
2. Precipitation reduces the near-surface concentration of mobile D in solution at low T.
3. Fractional occupation σ of traps in equilibrium with concentration C_s : smaller at high T.
   $$\frac{\sigma}{1-\sigma} = \frac{C}{z-C} \exp\left(\frac{Q_t}{kT}\right)$$
4. Saturable traps fill by diffusion from the near-surface:





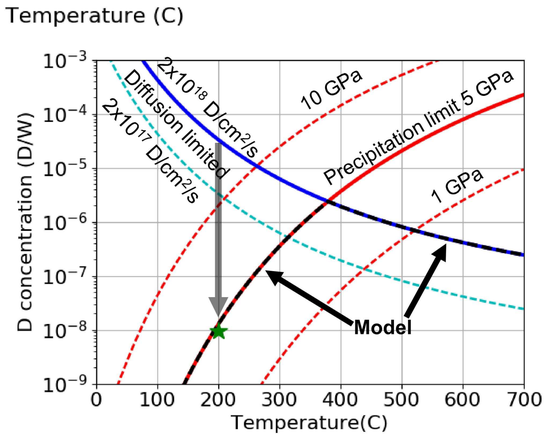
Pressure required for void growth by dislocation production is P_{max}~ µb/r ~ 1 - 10 GPa for r = 40 - 4 nm.

Corresponding concentration of D in solution is higher at higher T, $C_{max}=S\,(P^*_{max})^{1/2}$, where solubility $S=S_0\exp(-Q_s/kT)$.

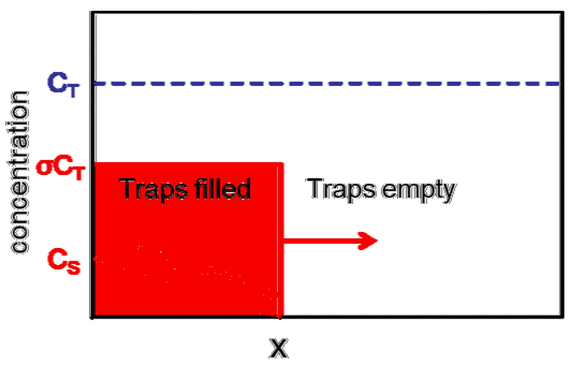
Pressure P and fugacity P* are related by the equation of state, P~P* for P<0.1GPa (ideal gas EOS PV=RT).

If C > C_{max} , D will flow into voids increasing their volume by plastic deformation, i.e. precipitates as molecular D_2. Voids may vent to the surface. Nucleation depends on microstructure.

Precipitation limits the D chemical potential, and the concentration of D in solution and traps, and the permeation rate to greater depths and overall D retention.



Kinetics



Flux to moving interface:

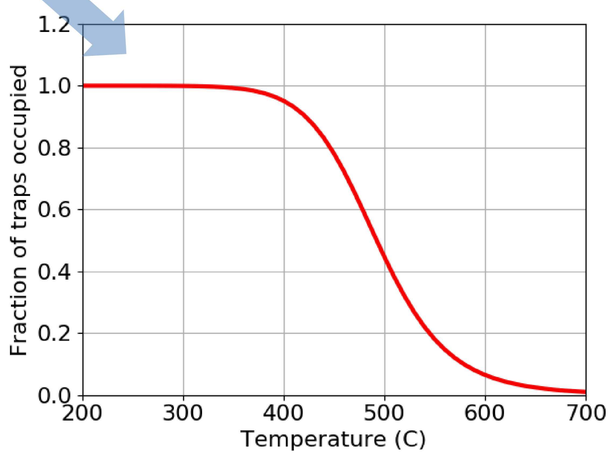
$$D\frac{C_s}{x} = \sigma C_t \frac{dx}{dt}$$

Depth to which traps are filled: (uniform trap concentration)

$$x = \sqrt{2Dt\frac{C_s}{\sigma C_t}}$$

Trapped D:

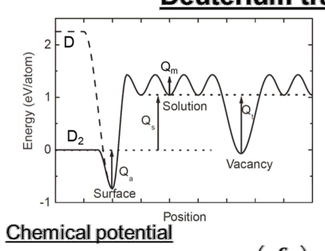
$$N_D = \sigma C_t N_W \, x = N_W\sqrt{2DtC_s\sigma C_t}$$



Φ=$2x10^{18}$/cm^{2}s, Q_t=1eV

1 eV traps are not effective above ~ 500°C

Deuterium trapping & precipitation - Energetics



Trapping: D bound to vacancy
Precipitation: formation of gas from solution
Enthalpies:
Q_m = 0.39 eV migration
Q_s = 1.04 eV solution
*Frauenfelder JVST **6** (1969) 388*
$Q_d = Q_t + Q_m$ =1.43 eV dissociation from trap
Q_t = 1.04 eV binding to trap (vacancy)
*Eleveld and Van Veen, JNM **191-194** (1992) 433*

Chemical potential

solution $\mu_s = H_s - T\,S_s + kT\ln\left(\frac{C}{z-C}\right)$

traps $\mu_t = H_t - T\,S_t + kT\ln\left(\frac{\sigma}{1-\sigma}\right)$

gas $\mu_g = \frac{1}{2}\left[H_g - T\,S_g + \int_{P_o}^{P} VdP\right]$

$= \frac{1}{2}\left[H_g - T\,S_g + kT\ln\left(\frac{P^*}{P_o}\right)\right]$

Fugacity (= pressure for ideal gas)

$$\frac{P^*}{P_o} = \exp\left(\frac{1}{kT}\int_{P_o}^{P} VdP\right)$$

with V from equation of state for D_2
Tkacz and Litwiniuk, J. Alloys and Compounds, 330-332 (2002)89.

Equilibrium when chemical potentials are equal:

Gas-solution

$$\frac{C}{z-C} = \sqrt{\frac{P^*}{P_o}}\frac{S_o}{z}\exp\left(-\frac{Q_s}{kT}\right)$$

S_0(P_o=1MPa) ~0.03 D/W

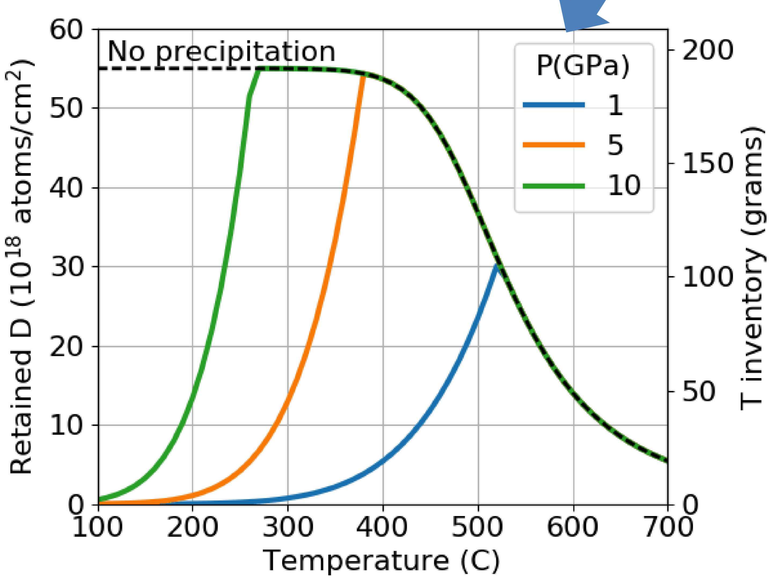
Solution-trap

$$\frac{\sigma}{1-\sigma} = \frac{C}{z-C}\exp\left(\frac{Q_t}{kT}\right)$$

z=6 solution sites per metal atom for bcc lattice, single trap occupancy, $S_s = S_t$

Gas-trap

$$\frac{\sigma}{1-\sigma} = \sqrt{\frac{P^*}{P_o}}S_o\exp\left(-\frac{Q_s}{kT}\right)\exp\left(\frac{Q_t}{kT}\right)$$



Example:
Estimated tritium inventory in ITER
Flux=2E18 D/cm^{2}s
Exposure time=$2x10^7$ sec (ITER end of life)
Trap concentration=0.002 traps/W
Binding energy to traps Q_t=1eV
50%T, 140 m^2 tungsten

DT retention is limited by slow permeation due to near-surface precipitation at T<300°C, and by binding to trap at T>500°C.

Conclusions

- **D in solution from implantation at high flux and low temperature has high chemical potential which drives precipitation and permeation.**
- **Precipitation reduces the near-surface D concentration in solution and hence the permeation to greater depths and overall D retention at lower temperatures.**
- **D retention at T<200°C is small due to slow kinetics, ie. permeation.**
- **D retention at T>500°C is small mainly due to weak binding to traps, not to defect annealing.**
- **D retention is high for 300 < T < 500°C where traps fill and permeation is fast enough to extend to greater depths.**
- **The model for D retention presented here includes effects of trapping and precipitation, and the dependence on incident flux & energy, exposure time & temperature, trap strength, needed for extrapolation to other conditions (eg. ITER).**

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