The Abdus Salam
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IAEA
International Atomic Energy Agency

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Plasma-Wall Interaction in Magentic Fusion
Recombination, Implantation, Diffusion and Release

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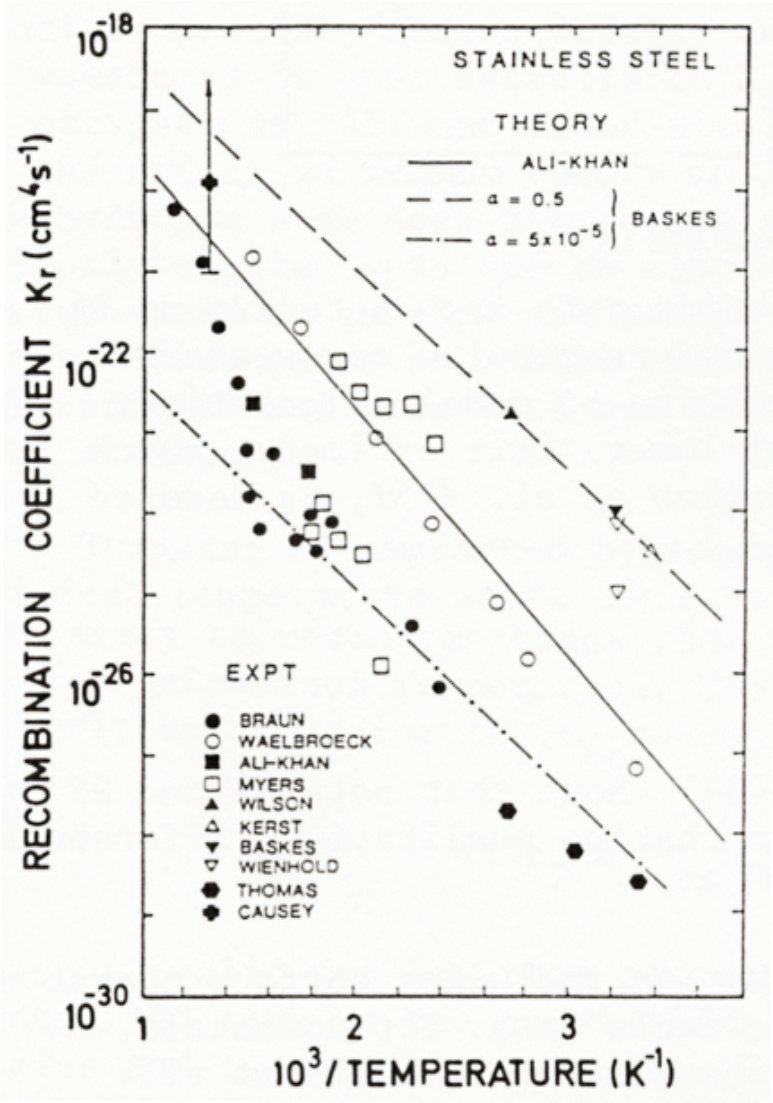
recombination, implantation, diffusion and release

heat load issues

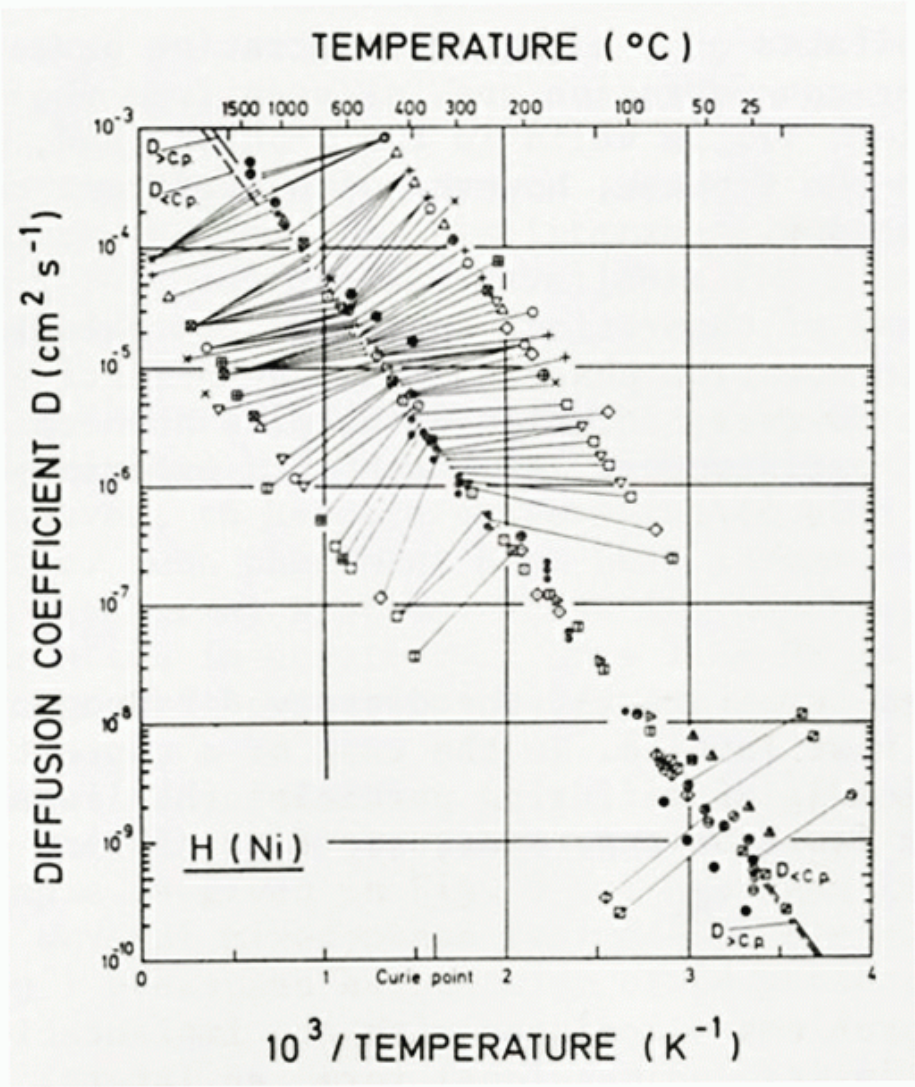
Recombination coefficient



Recombination coefficient for hydrogen in stainless steel

- acceptable data situation
- strong influence on surface conditions

Diffusion coefficients



- For many metals very detailed data exist for the diffusion of hydrogen
- However, data are very scarce for the potential first wall materials W and Be
- as well as for non-metallic compounds

H in metals

- hydrogen forms interstitial solution in metals
- small size of hydrogen, tunneling: very high mobility
- tungsten: low solubility of hydrogen
  - $\leq 10^{-8} - 10^{-6}$ at. fraction in perfect lattice
  - max. $\sim 10^{-3}$ at. fraction in defect-rich substrates
- tungsten as first wall material in fusion experiments (or reactors):
  - ion implantation (non-equilibrium)
  - high hydrogen fluence and flux
  - large first wall area
  - potentially large tritium inventory in first wall

thermodynamic treatment

- solubility and mobility of hydrogen in metal substrate
  - Determined by chemical potential $\mu_{metal}(\zeta)$
  - $\mu_{metal}(\zeta) = kT \cdot \ln\zeta + const.$ $\quad (\zeta = n_H / n_{sites} << 1)$

- equilibrium loading: e.g. from the gas phase
  - $Me + \frac{1}{2}x\ H_2 \rightleftharpoons MeH_x$
  - $\mu_{gas} = kT \cdot \ln(p/p_0) + const.$
  - Equilibrium condition: $\frac{1}{2}\mu_{Gas} = \mu_{Metall}$
- Sieverts‘ law for equilibrium concentration

  - $\zeta = K \cdot p^{1/2}$; $\quad K \propto \exp(-\Delta H_{sol.}/kT)$
  - Valid for single crystal, small concentration, ideal gas

- higher concentration $\Rightarrow$ higher equilibrium pressure

thermodynamic treatment

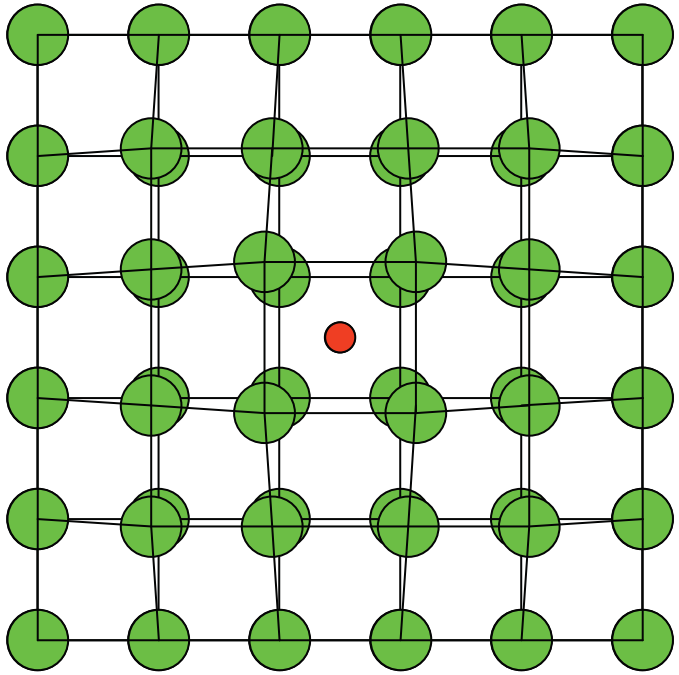
- μ can be **experimentally measured** (e.g. measurement of e.m.f)
  - Effective diffusion coefficient D_{eff}
  - Equilibrium concentration ζ

- sensity of states $n(E)$
  - determined by binding energies and concentration of sites for hydrogen
  - allows self-consistent calculation of μ
  - derivation of D_{eff}, ζ
  - modelling of hydrogen retention in tungsten

    macroscopic approach

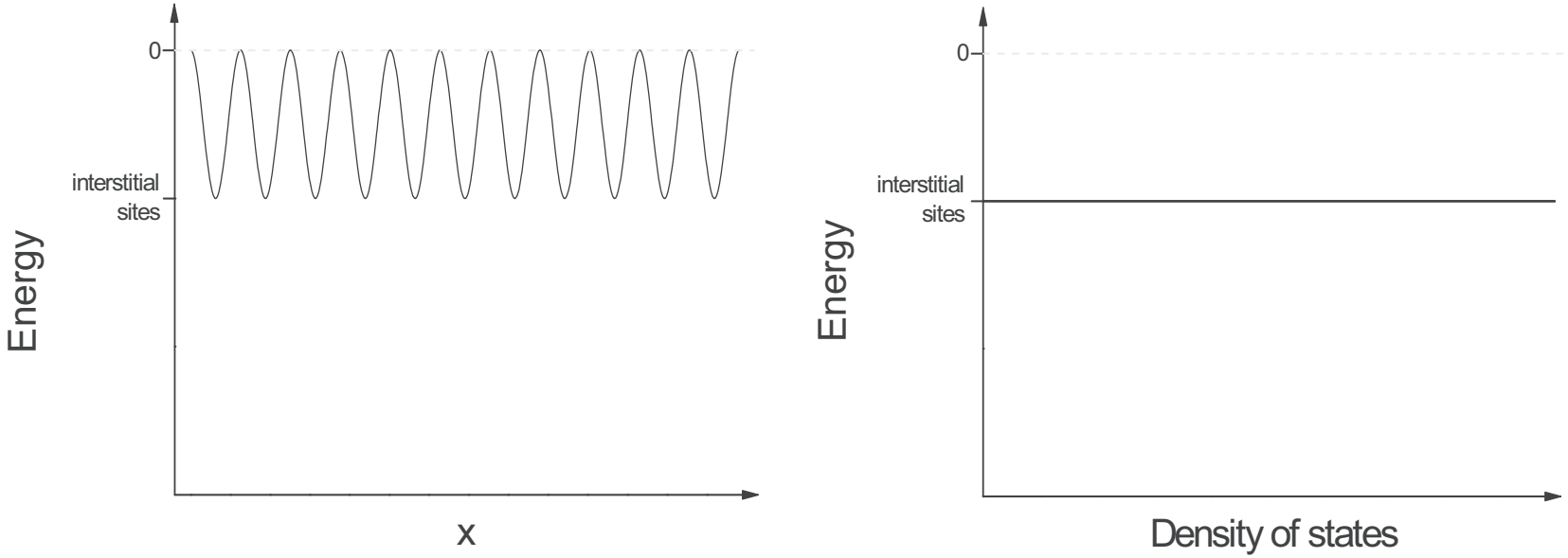
intrinsic defects

- perfect single crystal
  - „atomic“ hydrogen in interstitial sites
  - lattice distortion $\Rightarrow$ „self-trapping“



intrinsic defects

- perfect single crystal
  - energy diagram and density of states
  - diffusion coefficient by Frauenfelder [1]:
    - $D_{eff} = 4.1 \cdot 10^{-7} \cdot \exp(-0.39\ \text{eV} / k_{BT})$ m2/s
    - Interstitial binding energy (diffusion barrier) ~0.39 [1] eV

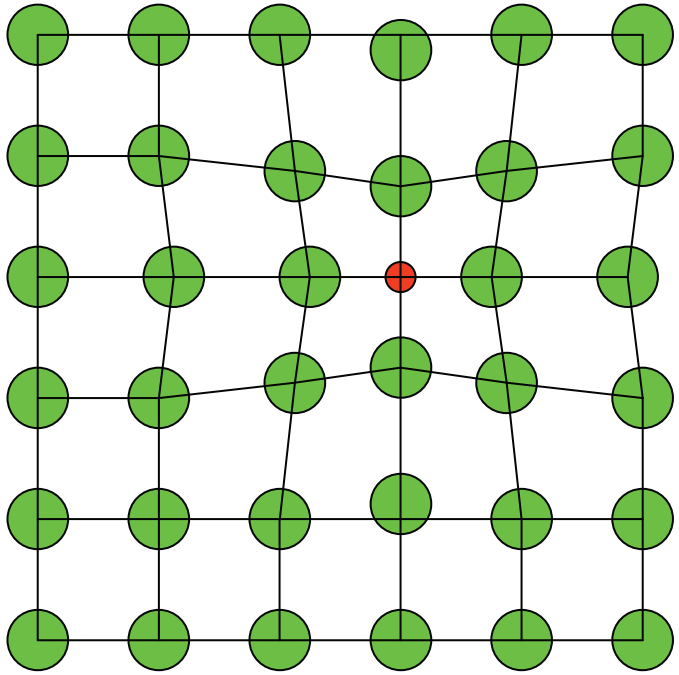


[1] R. Frauenfelder, *J. Vac. Sci. Tech* 6(3) (1968)

intrinsic defects

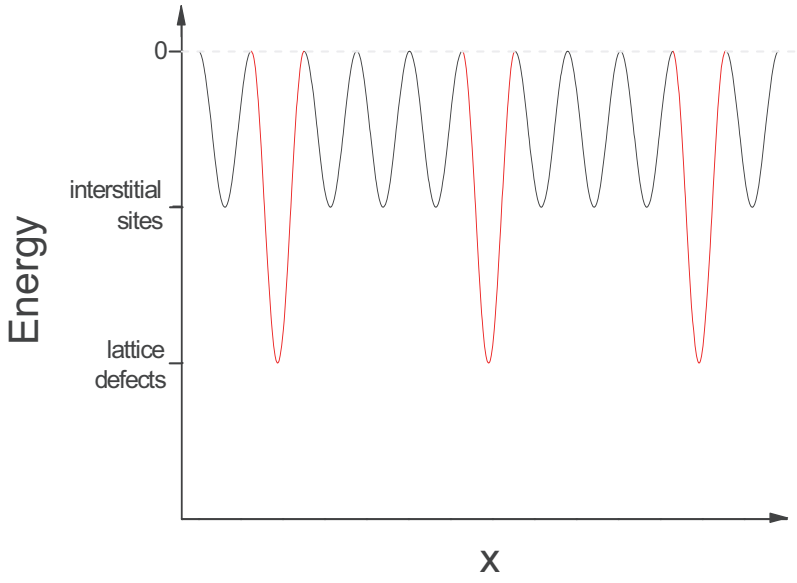
- point defects (vacancies)

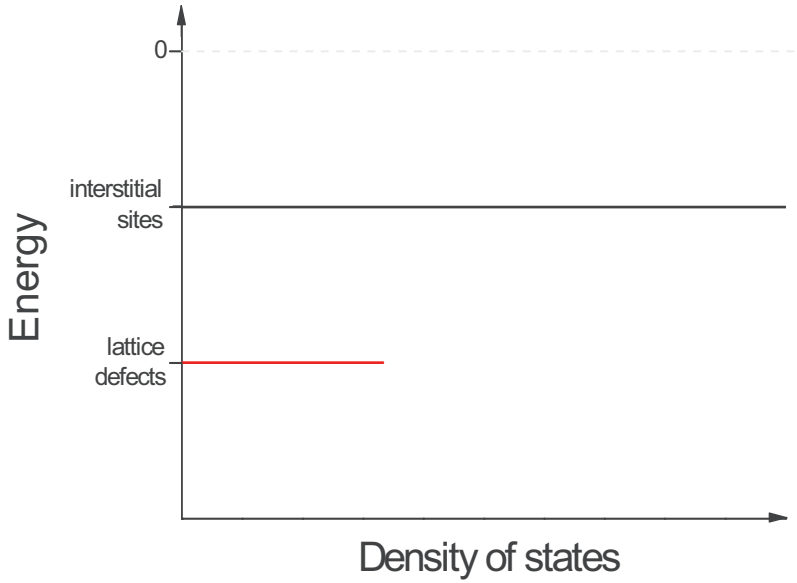
  concentration in thermal equilibrium $\propto \exp(-E_{vac} / kT)$



intrinsic defects

- point defects
  - strong binding of H atoms (E_b ~1.45 eV [1])
  - model: two-level system



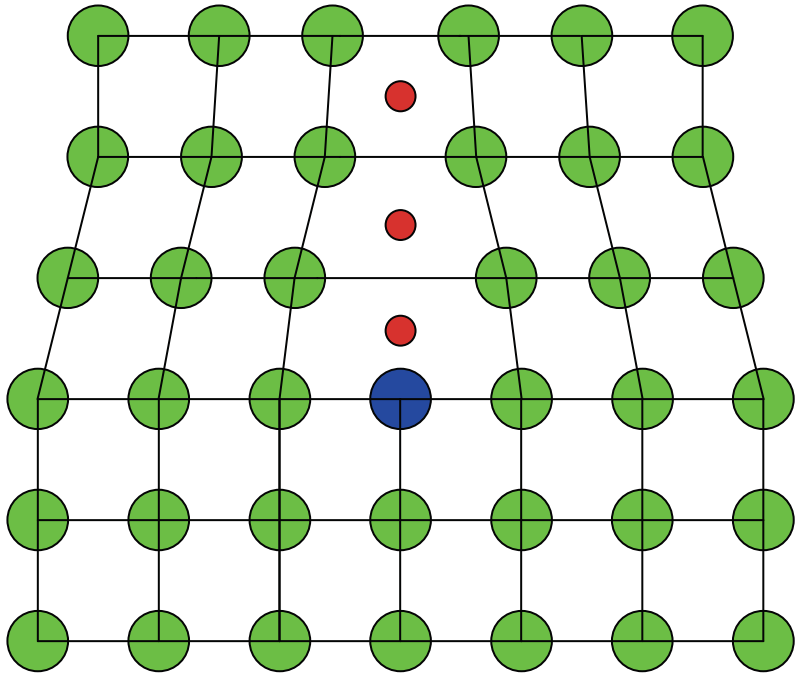


[1] O. Ogorodnikova, *et al.*, *J. Appl. Physics* 103 (2008)

intrinsic defects

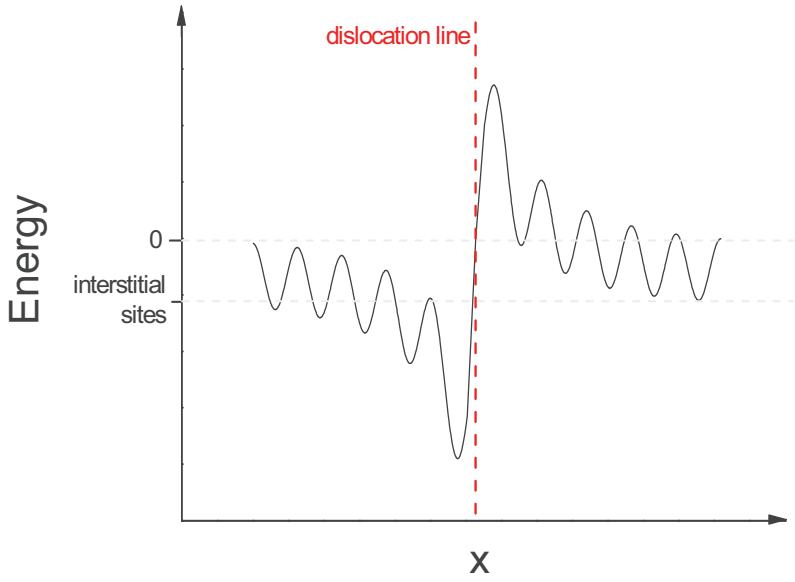
- dislocation lines

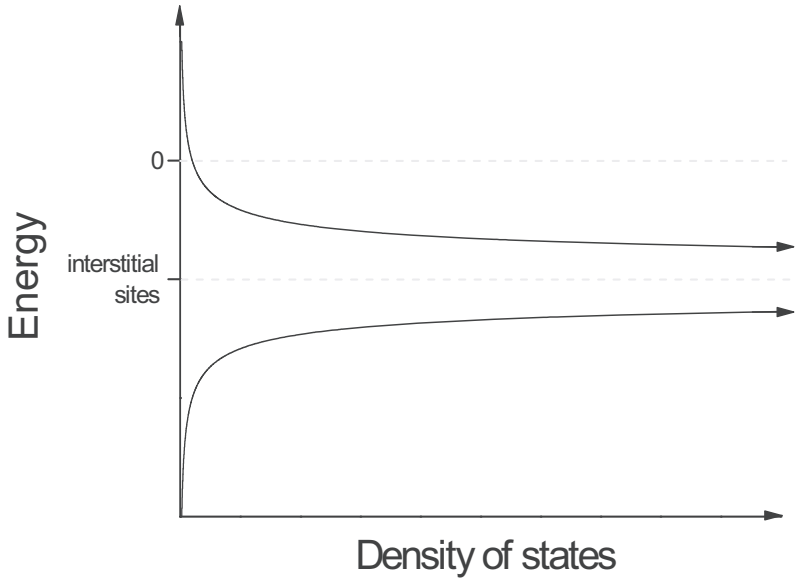
  long range elastic strain field also binds hydrogen



intrinsic defects

- Dislocation lines
  - Binding energy ~0,85 eV [1)]
  - Compressive side repulsive, tensile side attractive

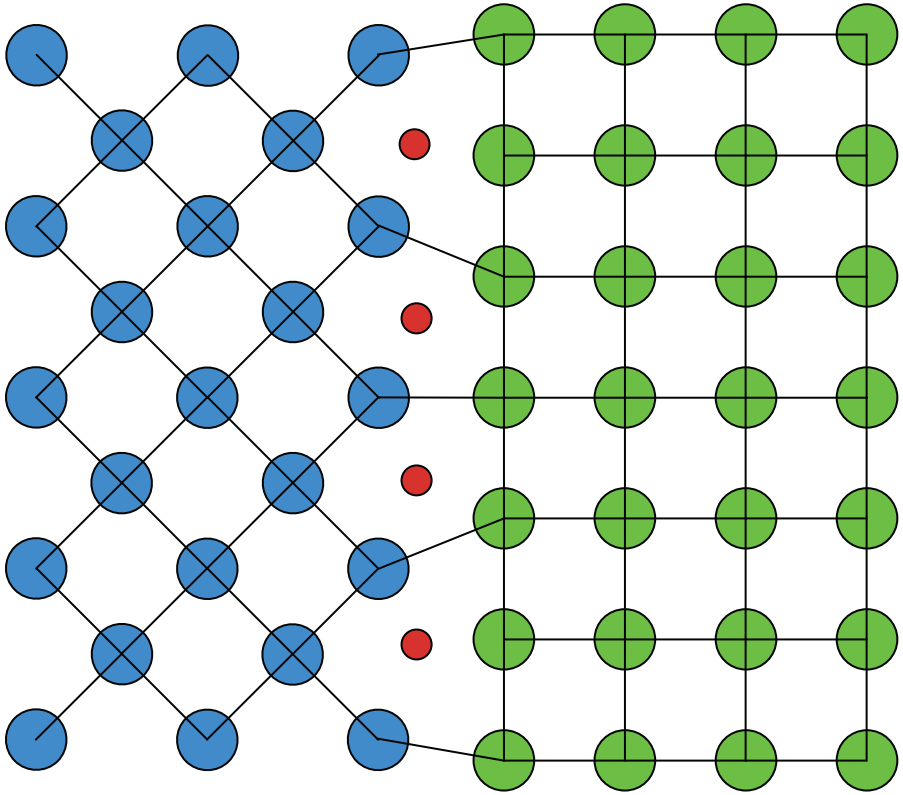




[1)] O. Ogorodnikova, *et al.*, *J. Appl. Physics* 103 (2008)

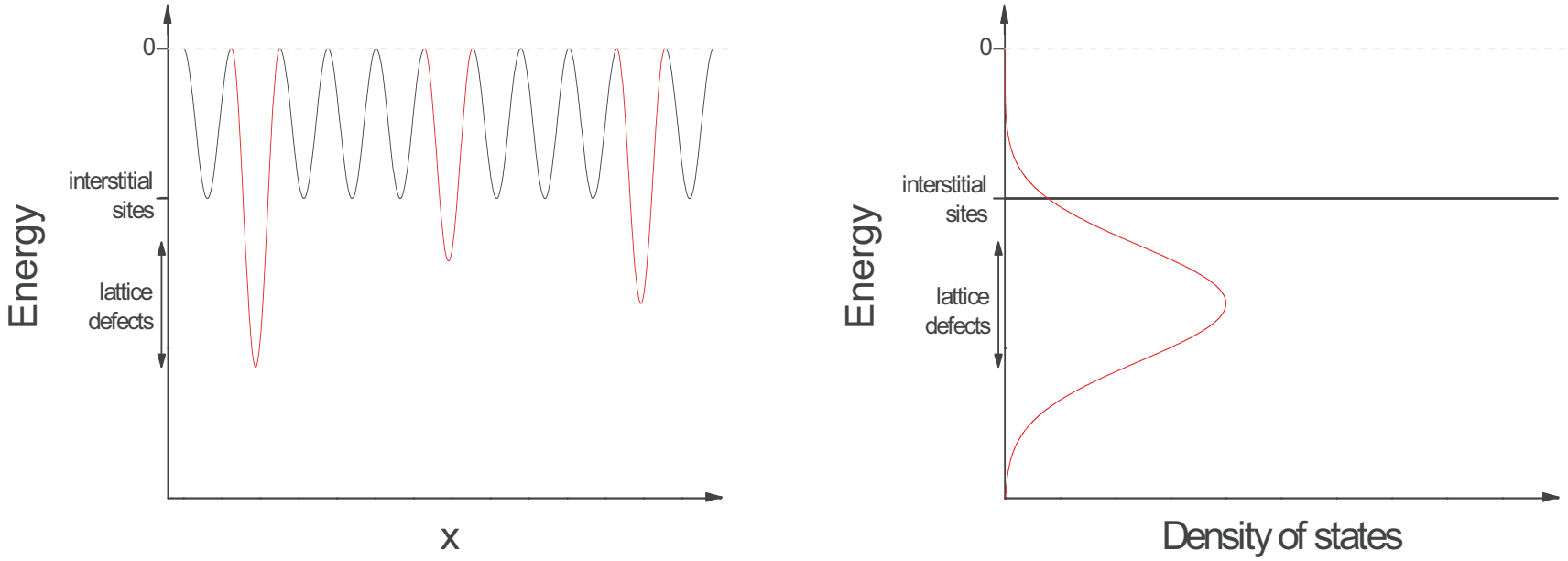
intrinsic defects

- Grain boundaries / phase boundaries
  - Mismatch between individual grains / phases
  - Size distribution of interstitial sites



intrinsic defects

- Grain boundaries / phase boundaries
  - Important for polycrystalline materials, deposited films, precipitations
  - Model: Gaussian distribution of site binding energies

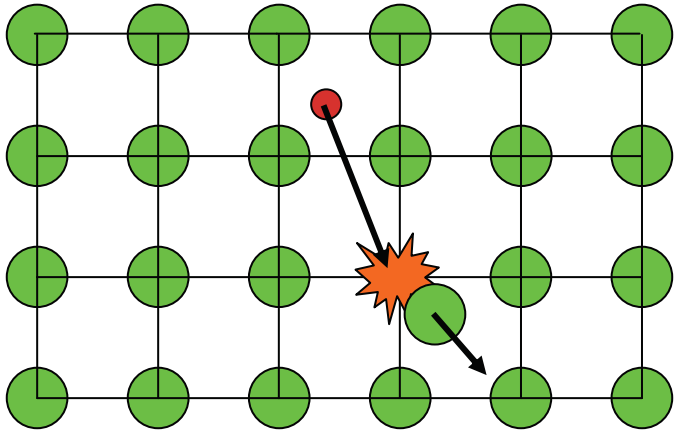


intrinsic defects

- three-dimensional defects
  - pores
  - cracks
  - binding energy ~1,45 eV [1)] (gaseous molecular H_2)
  - chemisorption on inner surfaces ~1,84 – 2,34 eV [1)]
- created also by ion implantation

extrinsic defects

- ion induced defects
  - elastic collisions of H with W $\Rightarrow$ point defects
  - only for high ion energies (keV)
  - within the stopping range of implanted ions (~10 – 100 nm)



extrinsic defects

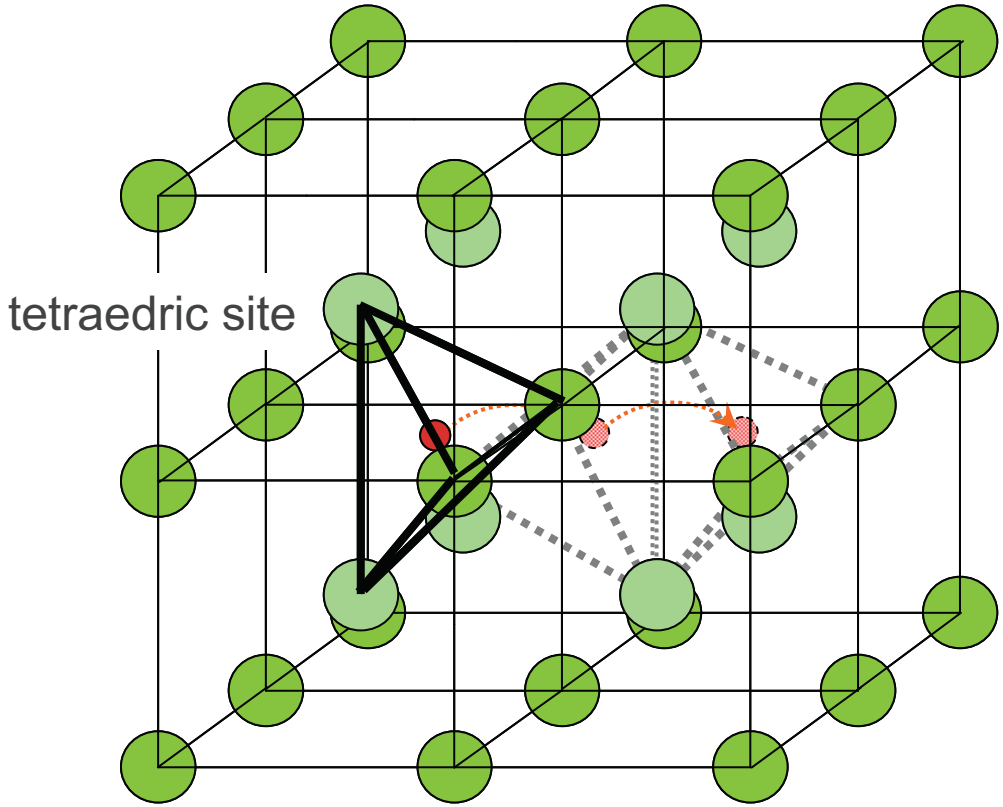
- other types of immediate radiation damage
  - creation and movement of dislocations
  - large strain on lattice in implantation region
  - created vacancies can form clusters
    - complex dynamic behaviour
    - growth, merging, annealing, annihilation
  - transition clusters $\rightarrow$ voids

extrinsic defects

- stress induced defects
  - non-equilibrium implantation
    - supersaturation
    - lattice strain
  - extremely high equivalent equilibrium pressure
    - plastic deformation
  - preferential accumulation of hydrogen at existing defects
    - positive feedback mechanism
  - creation and propagation of cracks
  - creation and growth of voids and bubbles
  - delamination of layers
  - blistering

transport mechanisms

- tungsten: **bcc** lattice
  - tetraedric interstitial sites larger ⇒ preferred sites for hydrogens
- jumps between neighbouring tetraedric sites

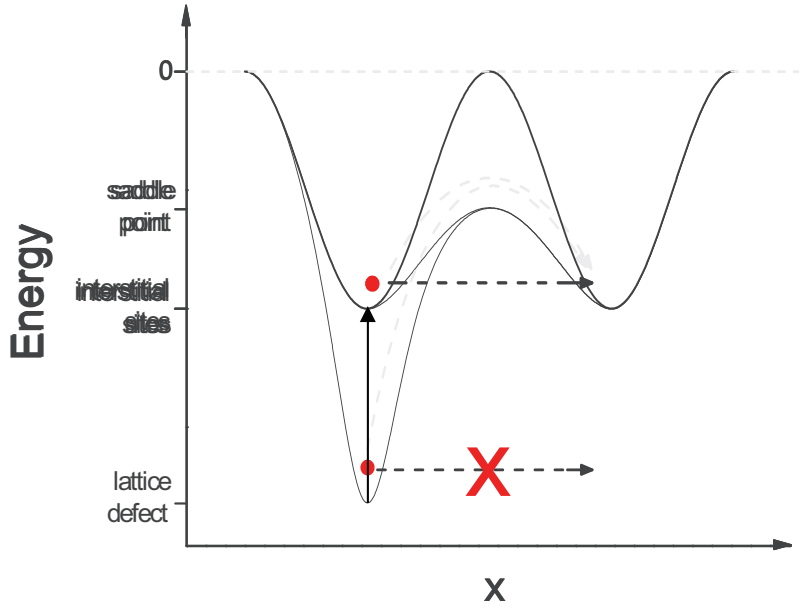


transport mechanisms

- small energy barrier between tetraedric sites
  - high mobility of hydrogen ($D_{eff} \sim 10^{-7}$ m^2/s)
    Corresponds approximately to D_{eff} of ions in aqueous solution
- diffusion mechanisms
  - quantum mechanical treatment necessary (tunnel effect)
    isotope dependence of tunneling cross section
  - room temperature:
    - self-trapping of H atoms $\Rightarrow$ „hopping“ to next neighbours
  - $T_{substrate}$ high:
    - thermal excitation over barrier; also long range jumps or intermittently „free“ atoms
  - $T_{substrate}$ very low:
    - coherent (band-like) tunneling theoretically possible
    - usually suppressed by impurities / lattice imperfections

transport mechanisms

- **thermally activated** tunneling
  - reduction of energy barrier between sites by lattice vibrations
  - transitions of H atoms into excited states
  - energetic leveling of neighbouring sites



transport mechanisms

- influence of extended defects
  - grain boundary diffusion
  - increased diffusion along dislocation lines
- „dislocation drag“
  - movement of dislocations
  - hydrogen bound to dislocation dragged along
- vacancy diffusion
  - diffusion of substituted hydrogen atoms through host lattice

transport mechanisms

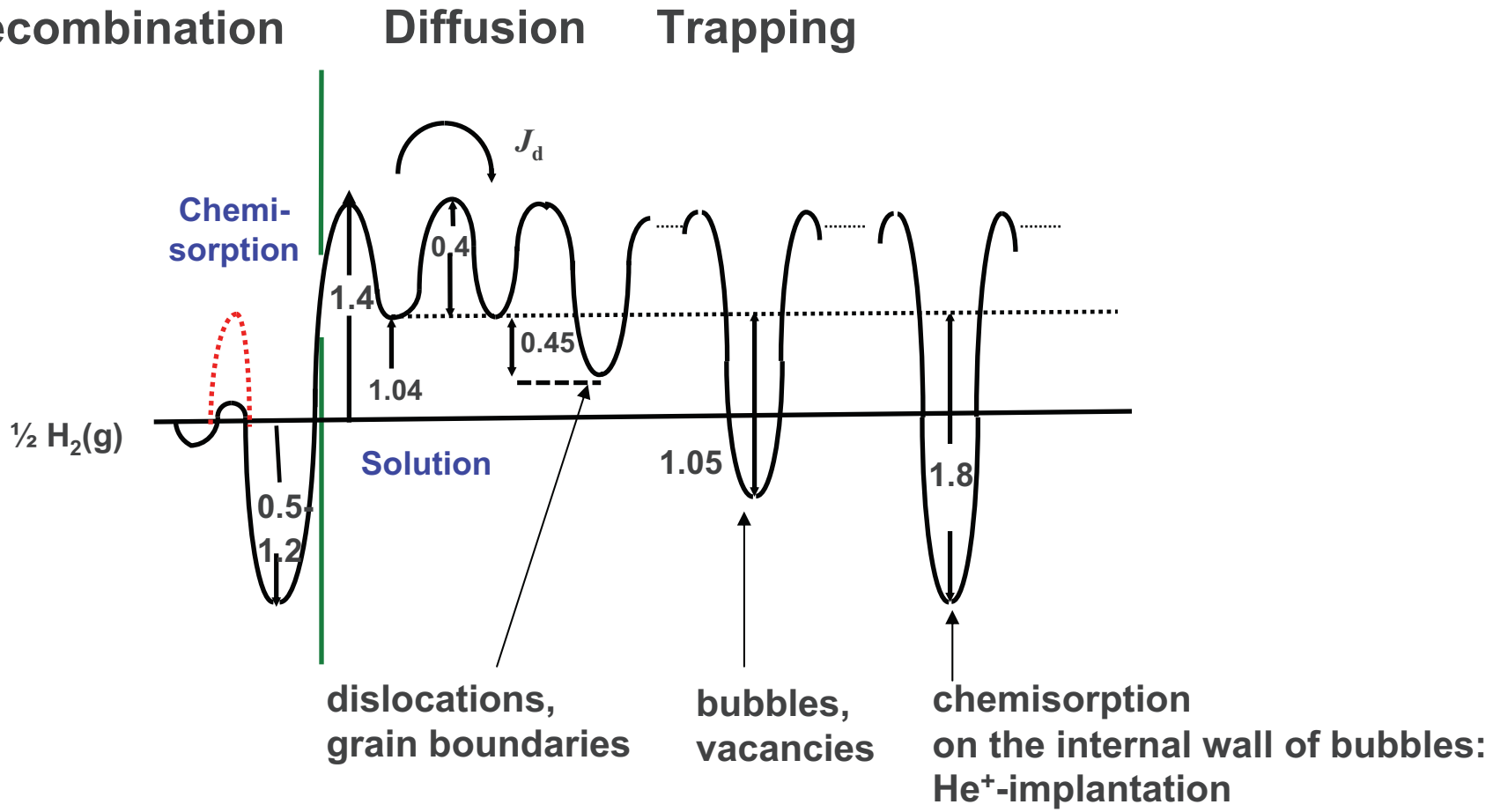
- „stress assisted diffusion“
  - interstitial hydrogen strains host lattice
  - hydrogen avoids external mechanical compressive stress
  - also caused by stress created in implantation region
  - migration of hydrogen into regions of tensile stress respectively less compressive stress
- other diffusion mechanisms
  - e.g. electromigration, thermotransport
- **directional** transport into bulk driven by gradients of
  - concentration
  - stress
  - temperature
  - electric potential

diffusion of H in W

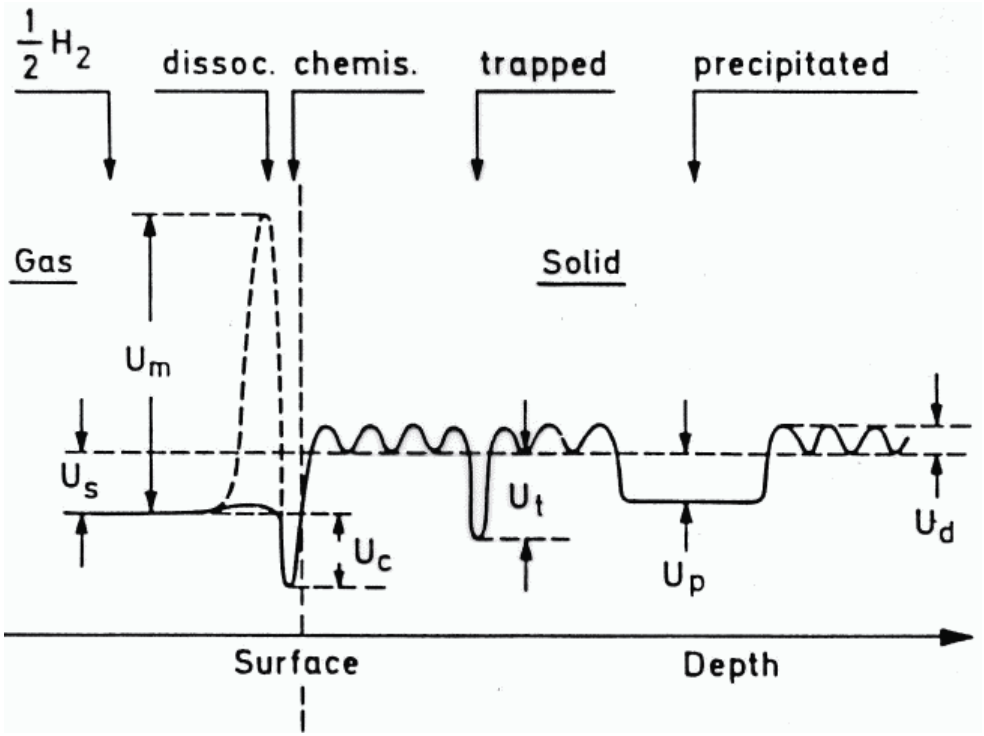
- high mobility, directed transport
  - deep penetration of hydrogen into substrate possible
- strong binding to defects
  - retention depth profile determined by defect density
- intrinsic defects
  - assumption: constant density averaged over volume >> a^3
  - implantation into δ-layer near surface

    exponential decay of retained hydrogen density into bulk
- extrinsic defects
  - locally increased defect density
  - peaks expected in depth profile of retained hydrogen

mechanism of deuterium behavior in polycrystalline W



schematic energy diagram for H in metals



Processes:

- Implantation, Diffusion, Trapping

$$\frac{\delta c_s}{\delta t} = D(t)\frac{\delta^2 c_s}{\delta x^2} + S(x,t) - T(c_s, c_t, x, t)$$

source term S from range distribution

$$D = D_0 e^{-\frac{U_d}{kT}}$$

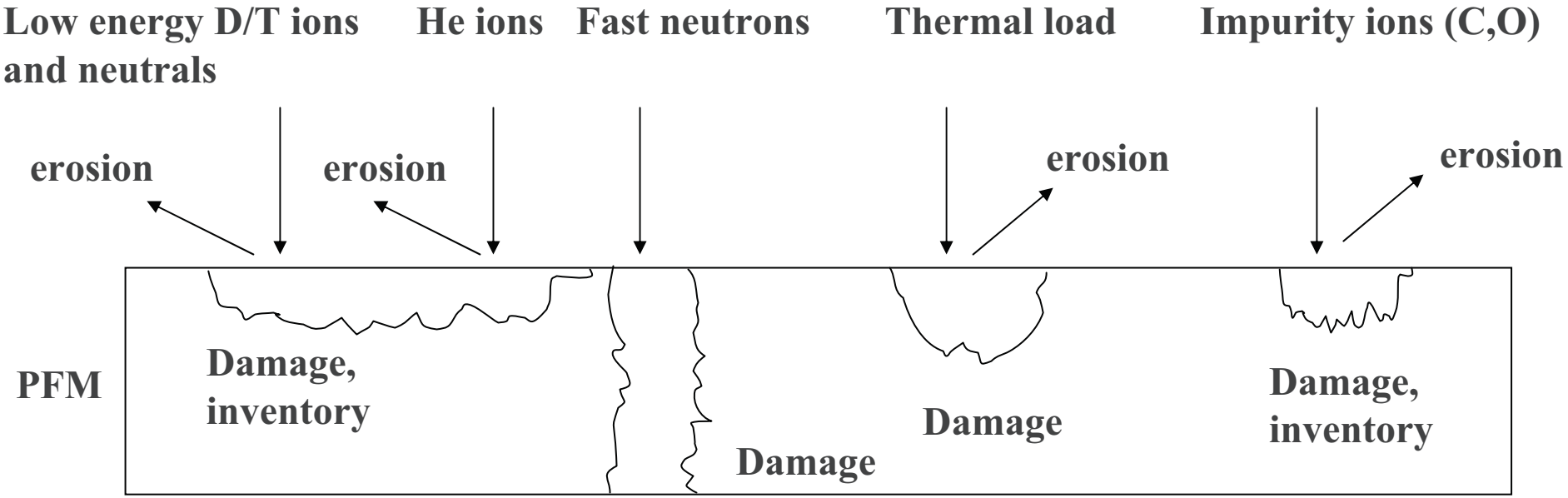
$$T = 4\pi r_d D\left[c_s\left(c_T - c_t\right) - N_H c_t e^{-\frac{U_t}{kT}}\right]$$

- Recombinative release

steady state fluxes $j_- = Kc_s(0)^2$, $j_- = Kc_s(d)^2$

K recombination constant $K = \frac{K_0}{\sqrt{T}} e^{-\frac{U_r}{kT}}$

inventory issues



1) Fatigue properties:
-bulk radiation damage by fast neutrons (vacancies, interstitial clusters)
-damage due to low energy ions and neutrals escaping the plasma
-thermal fatigue due to energy deposition
2) Thermal shock due to off-normal operation
3) corrosion

What do we want to know and which techniques are used?

Results needed:

diffusion and permeation of implanted atoms

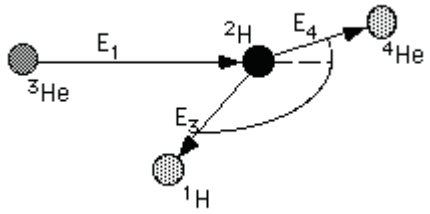
trapped D/T inventory

trap energy, i.e. temperature needed for desorption

Experimental techniques

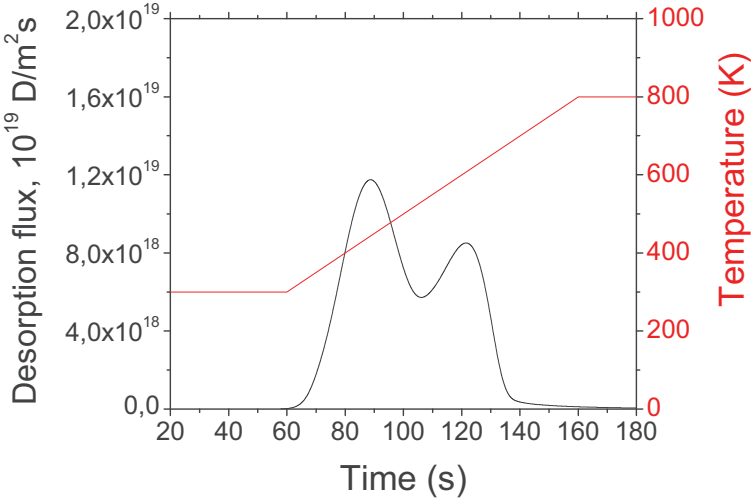
reemission and permeation experiments using upstream and downstream residual gas analysis.

depth profiling after implantation.

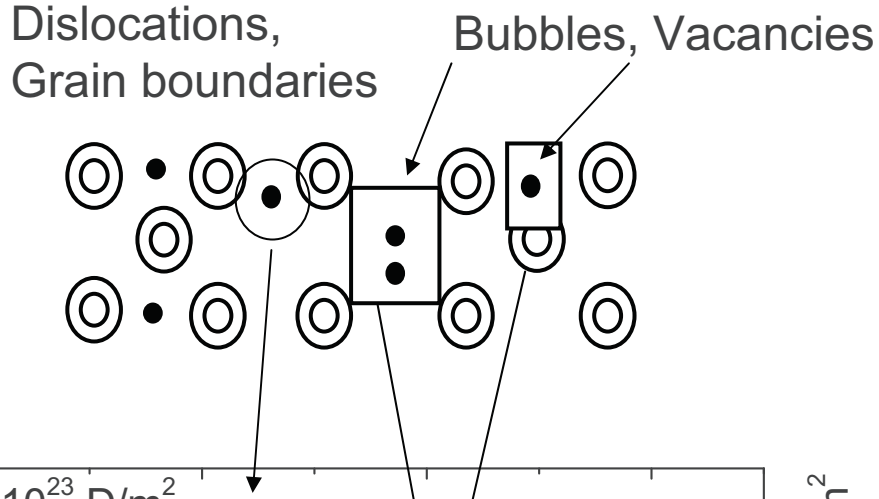


thermal desorption analysis.

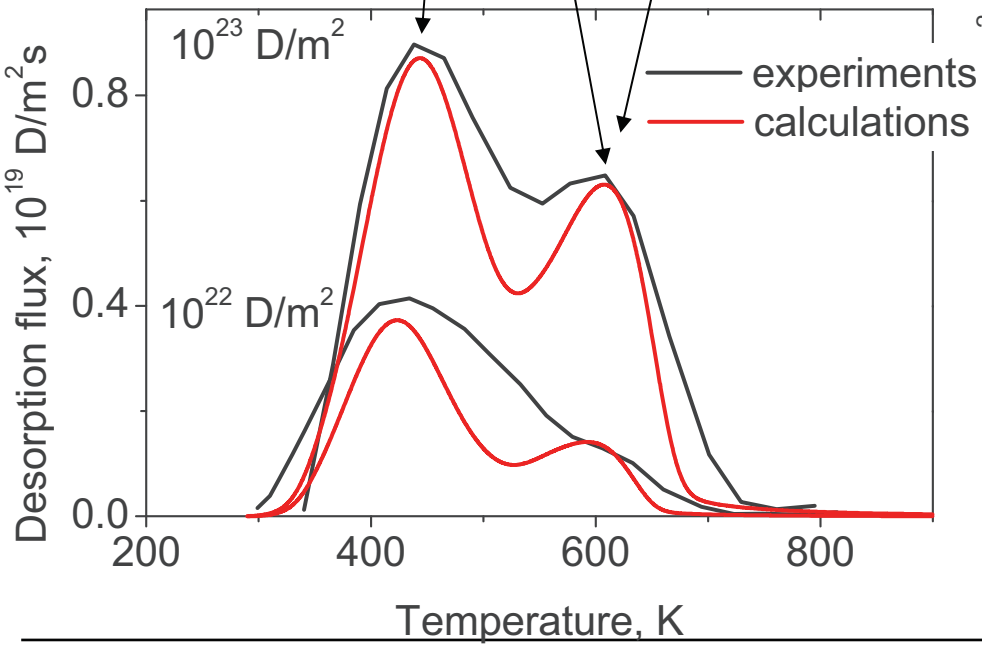
linear ramp thermal desorption experiments

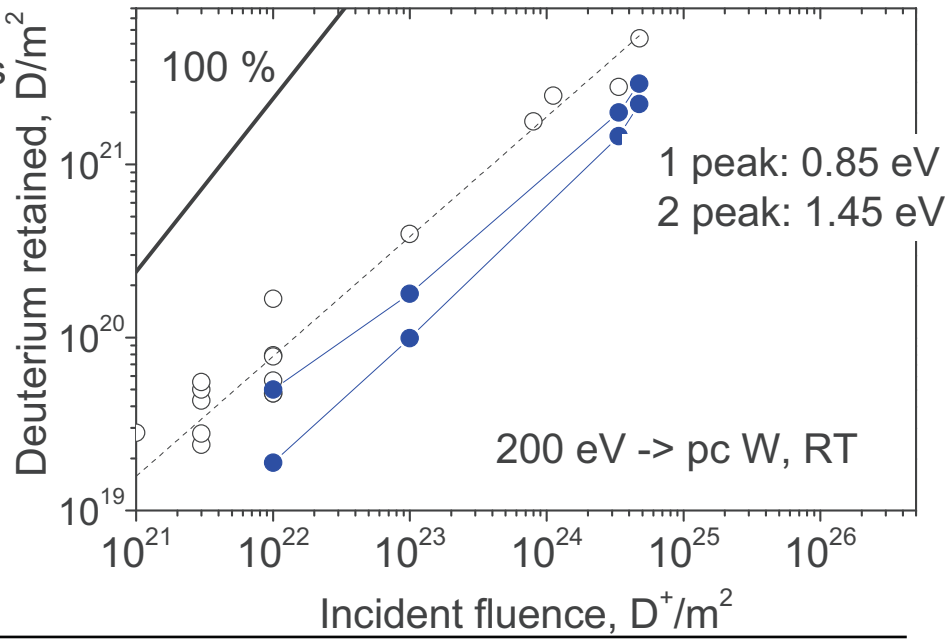


diffusion-limited trapping of deuterium in polycrystalline W



- the concentration of 1.45 eV traps increases during implantation
- the D retention in 0.85 eV traps increase with fluence because of diffusion

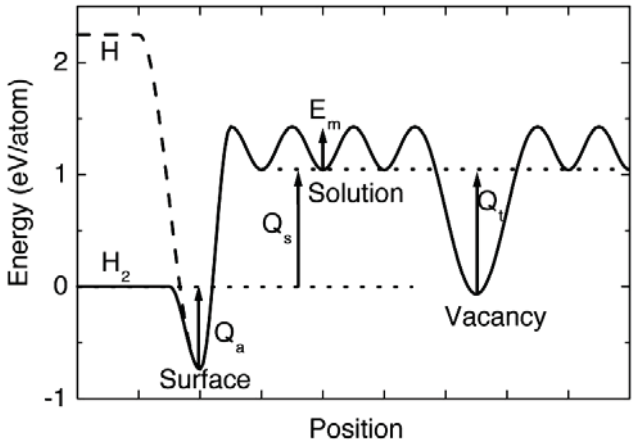




influence of surface impurities on retention

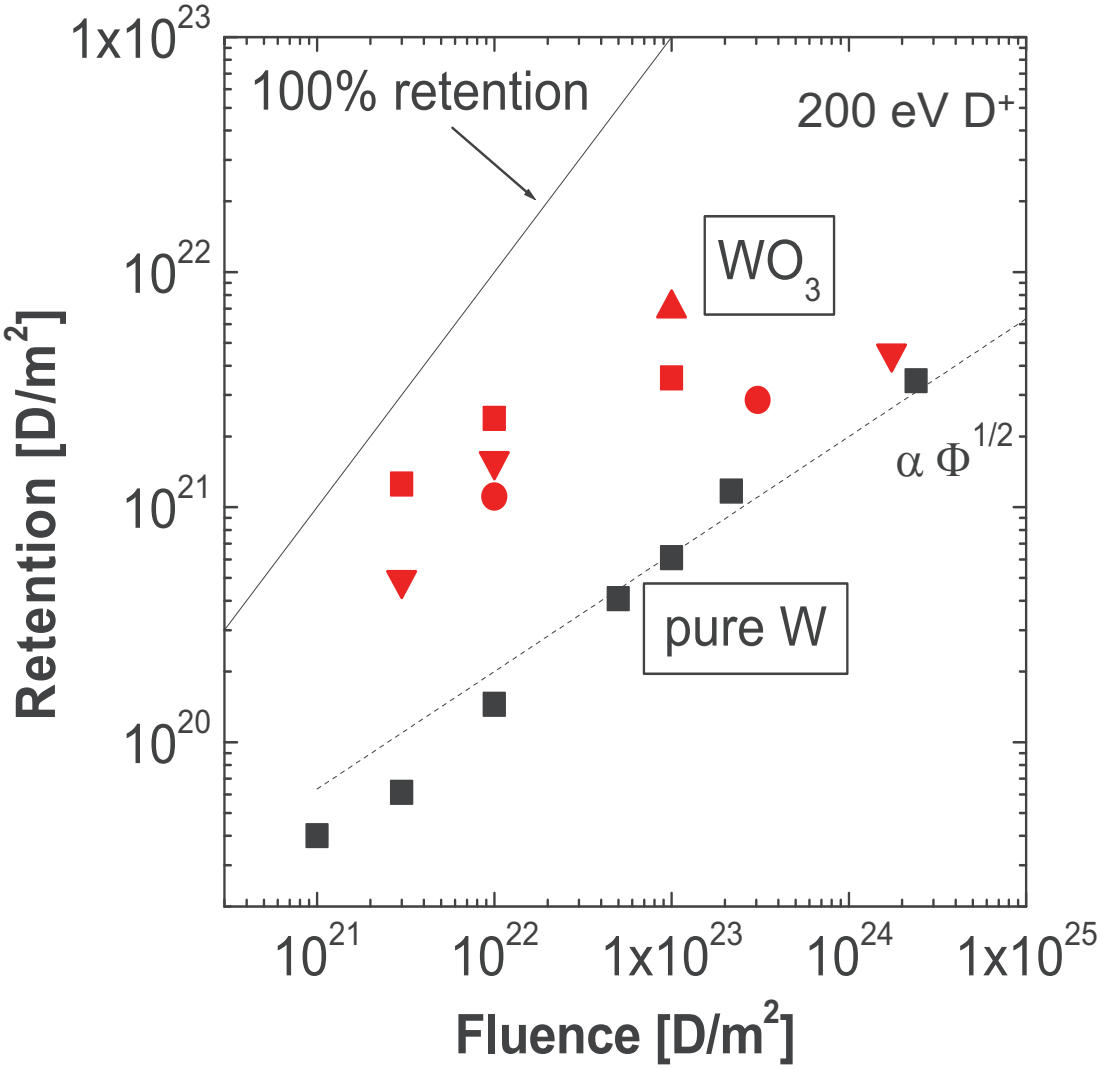
in tungsten:

retention dominated by diffusion and trapping

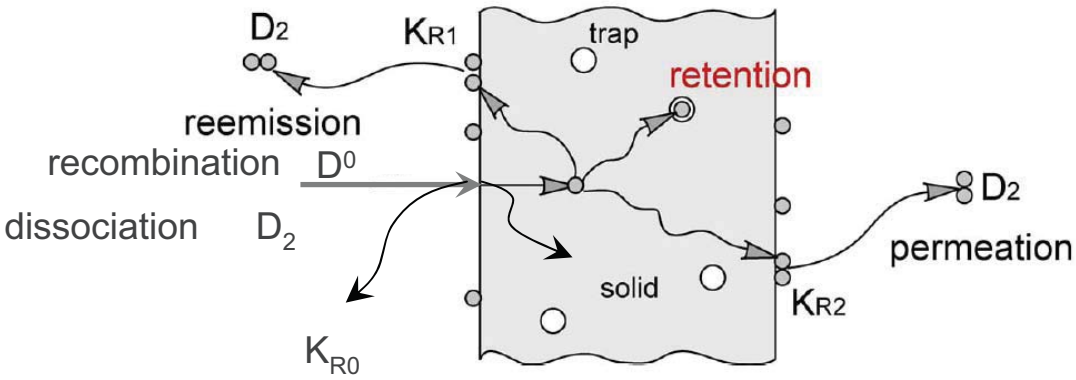


no saturation at high fluences

enhanced retention due to oxide and carbide surface layers



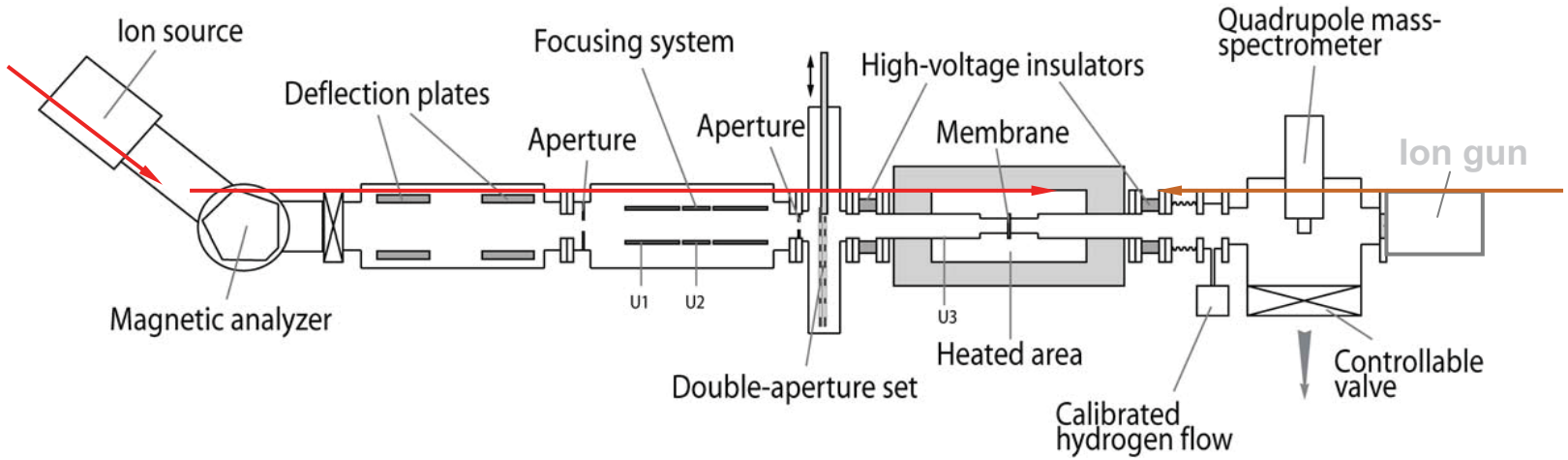
hydrogen permeation through metals

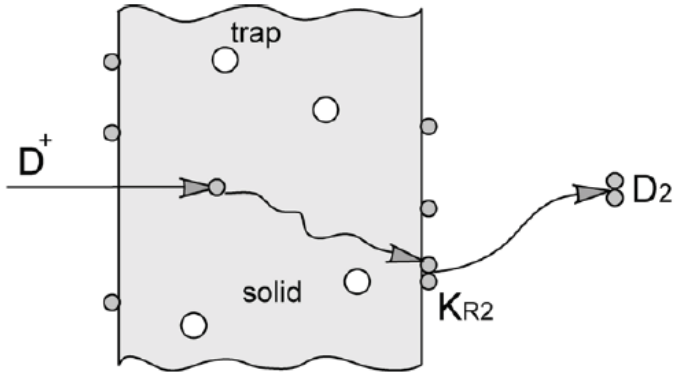


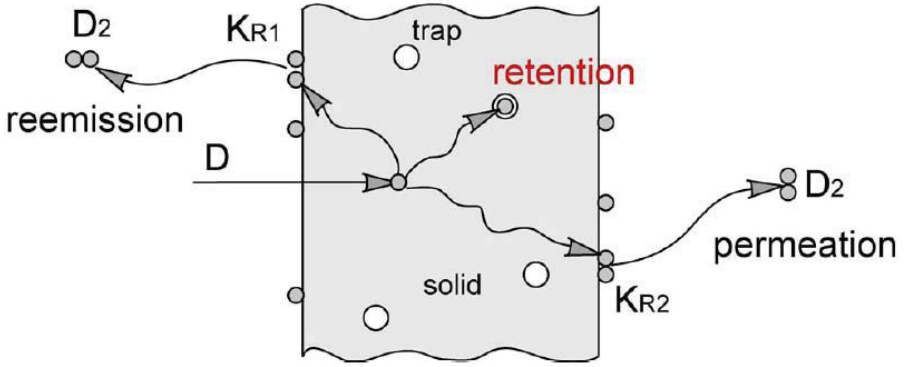
hughe influence of surface conditions!

ion driven permeation

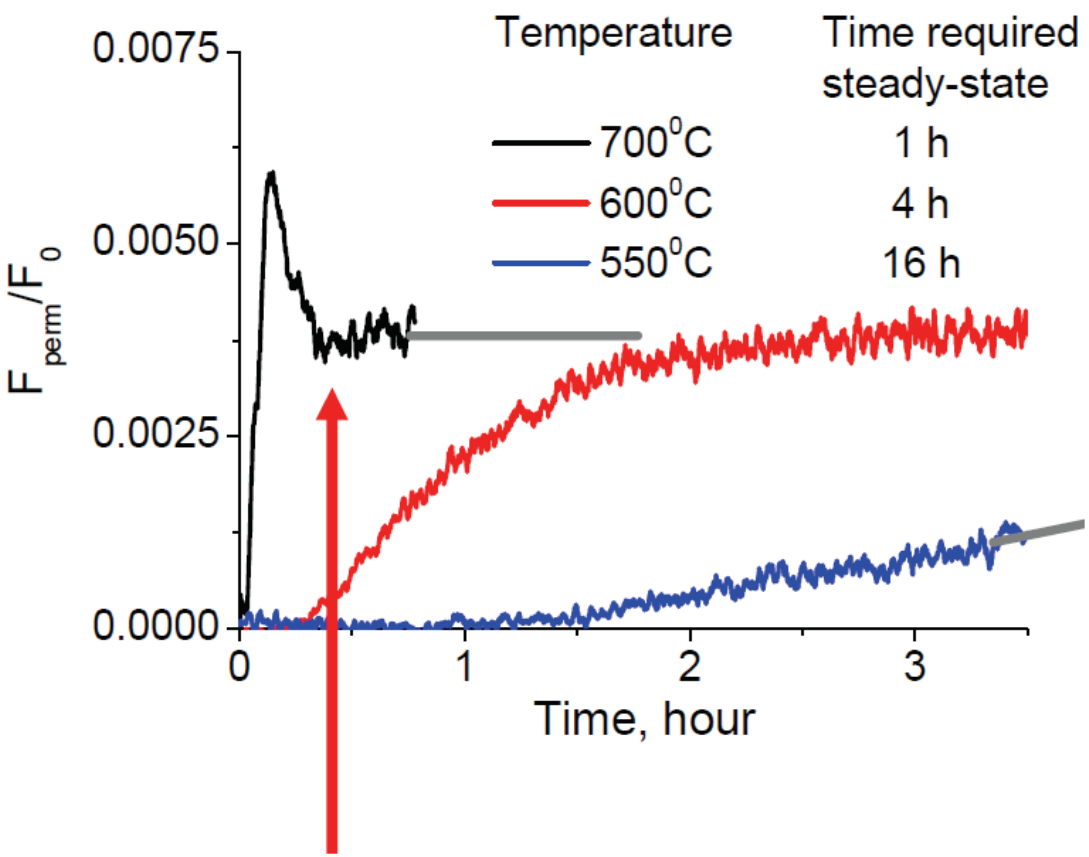
lab experiment PERMEX M. Mayer







ion driven permeation



A. Golubeva, M. Mayer

D (200 eV) =>

3 different samples
W 50 µm,

unknown producer
(grain sizes ~ foil thickness, so the diffusion along grain boundaries is a possible mechanism)

backsides of membranes were cleaned by Ar^+ (1.5 keV)

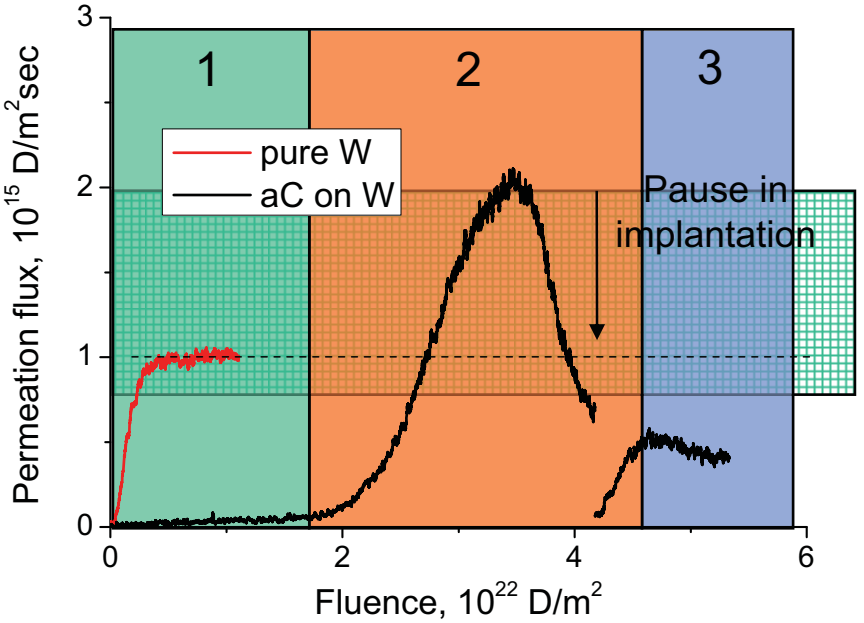
20 min – seems to be the time of impurities on front side sputtering
(Note: D (200 eV) does not create displacement defects in W)

ion driven permeation : influence of carbon layers

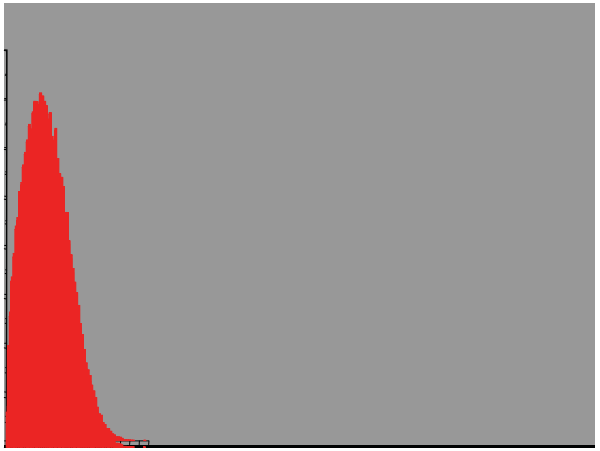
1 - Thick film. All deuterium stop inside the carbon film. No IDP

2 – Thin film – maximum of permeability

3 - “Clean tungsten”. The permeation flux is less than for pure tungsten experiments
probably implanted C as barrier



Strong influence of impurity layers on front side on permeation



Y. Gasparyan, M. Mayer

ion driven permeation : influence of carbon layers

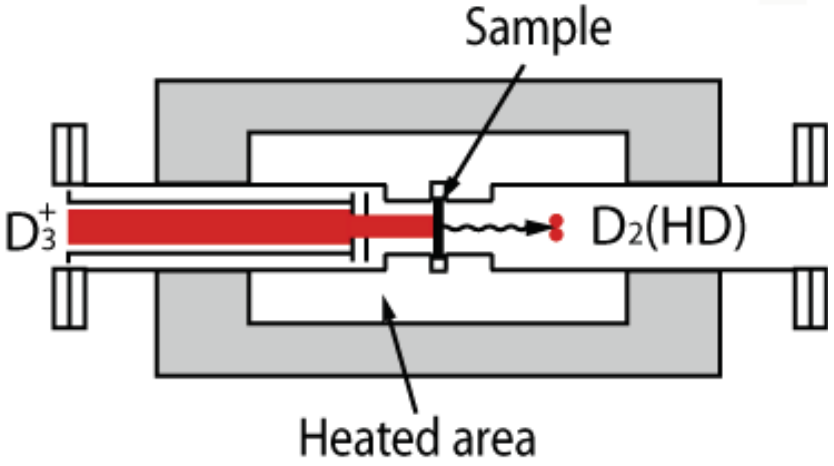
Temperature: 823 - 923 K

Ion energy: 200-3000 eV/D

Incident flux: ~10^{18} D/m^2sec

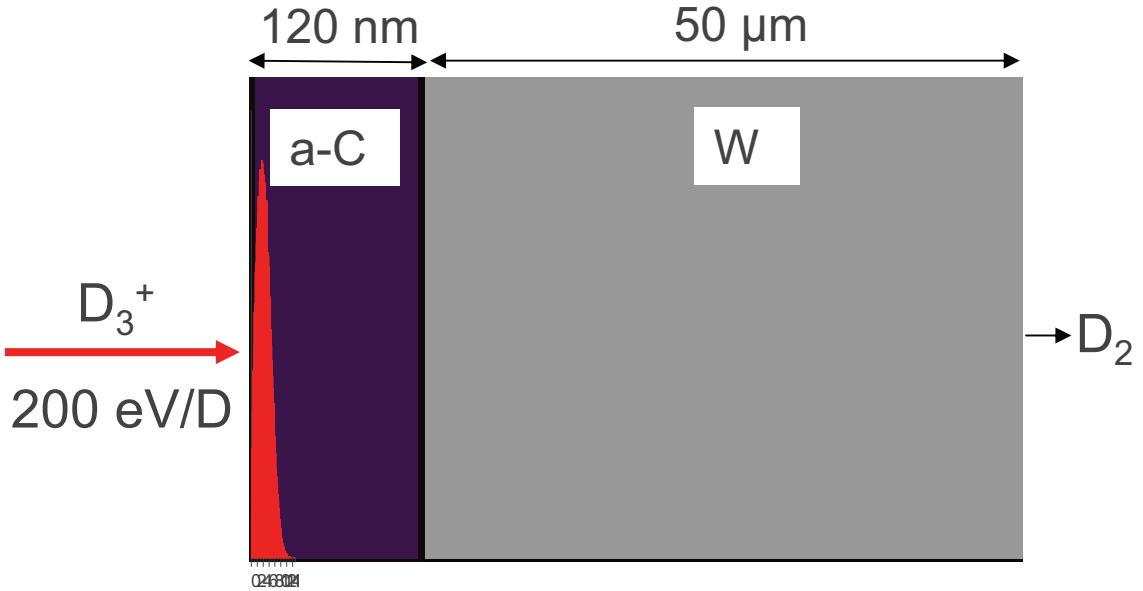
D_2 pressure: ~ 7×10^{-4} Pa

Sample thickness: 50-200 µm

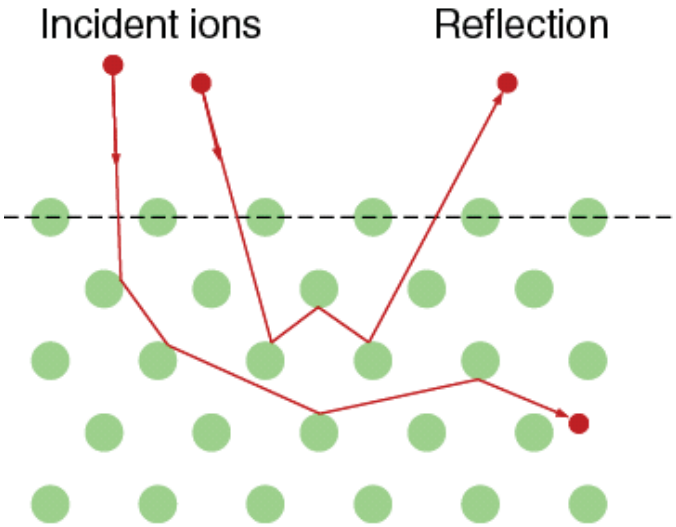


Sputter-deposited 120 nm
a-C layer on front surface

Y. Gasparyan, M. Mayer



hydrogen inventory - implantation



Trapping in grain boundaries and vacancies

⇩

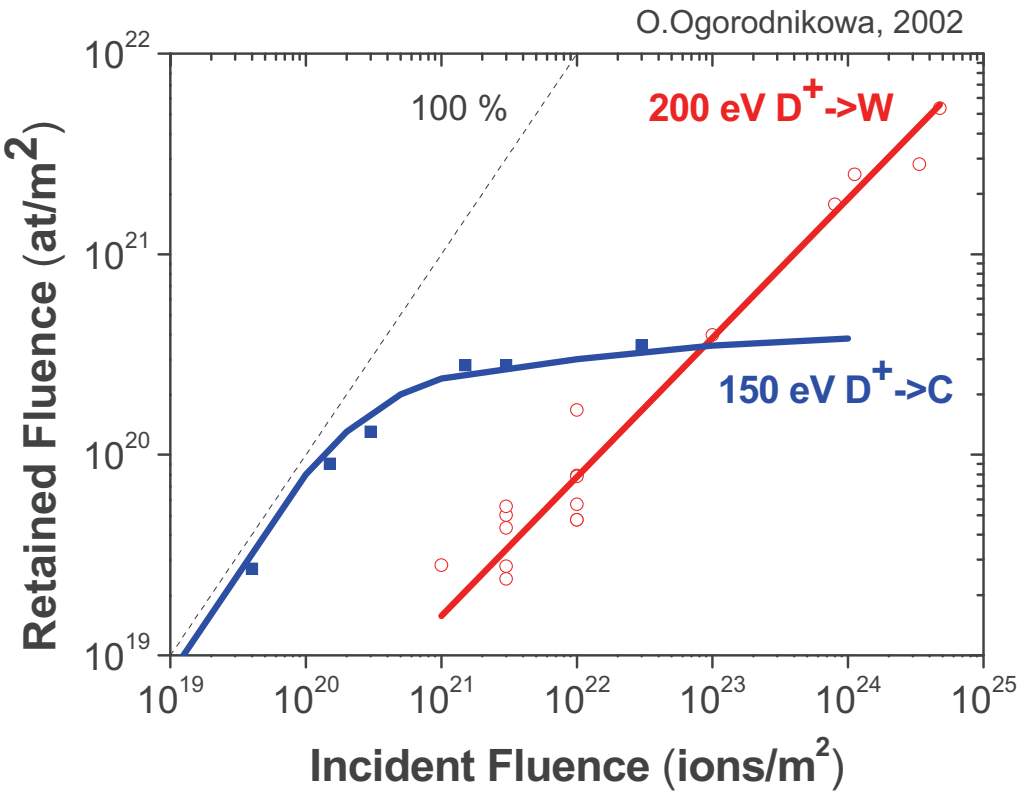
Diffusion ($\sim e^{-E_D/kT}$)

Recombination ($\sim e^{-E_R/kT}/\sqrt{T}$)

Thermal desorption

Be, W: <600K

C: ≈1500K



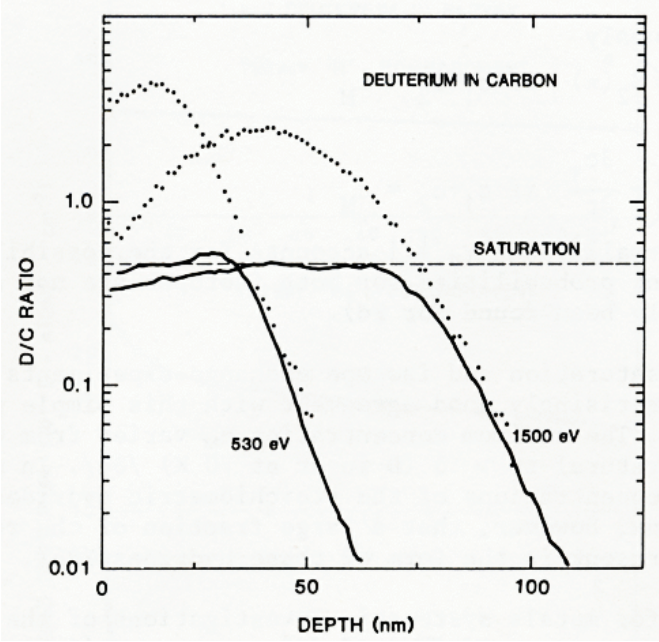
Hydrogen inventories are dominated by trapping at defects

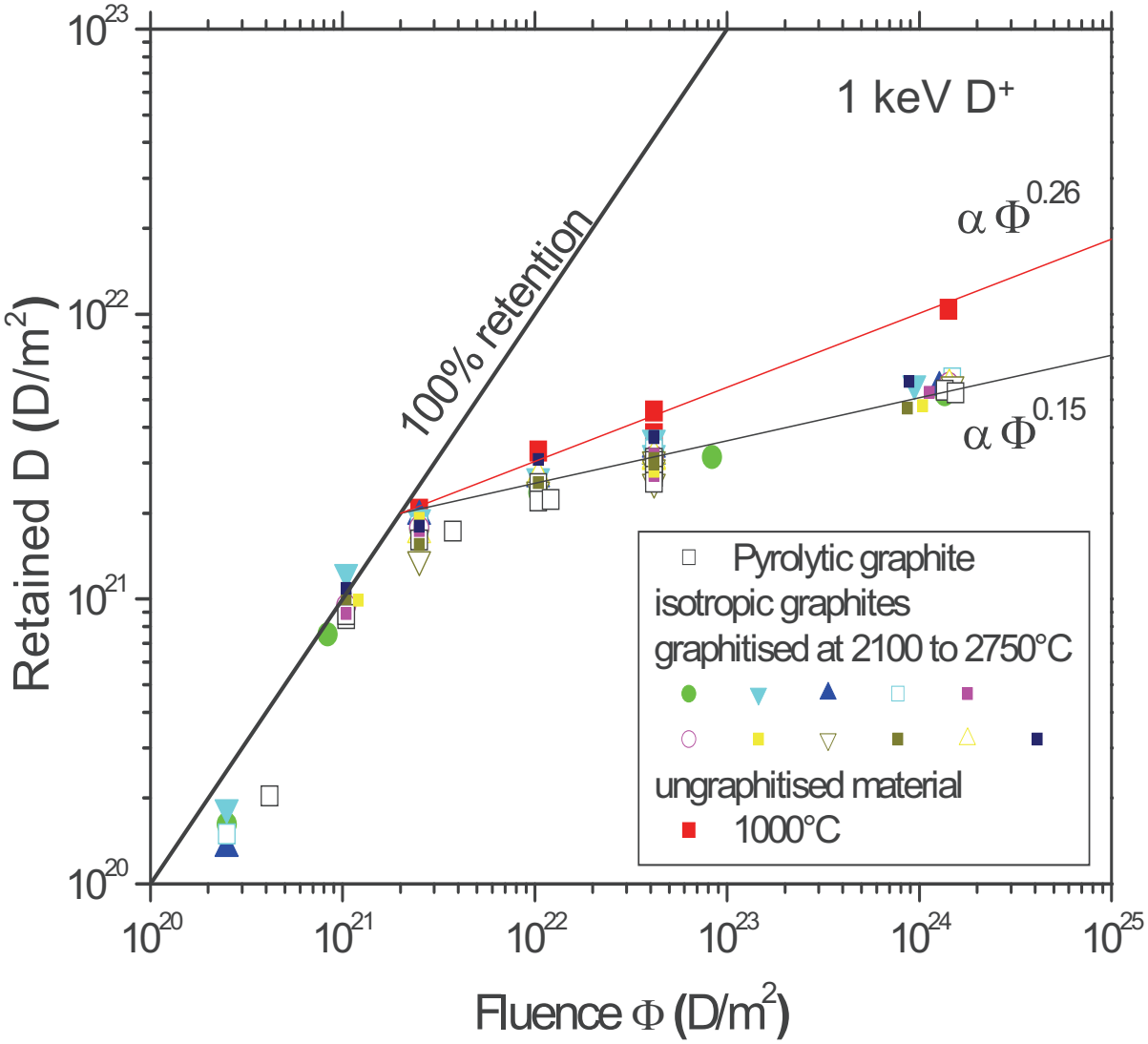
mechanisms of hydrogen retention in carbon

in carbon materials:

100% retention at low fluences

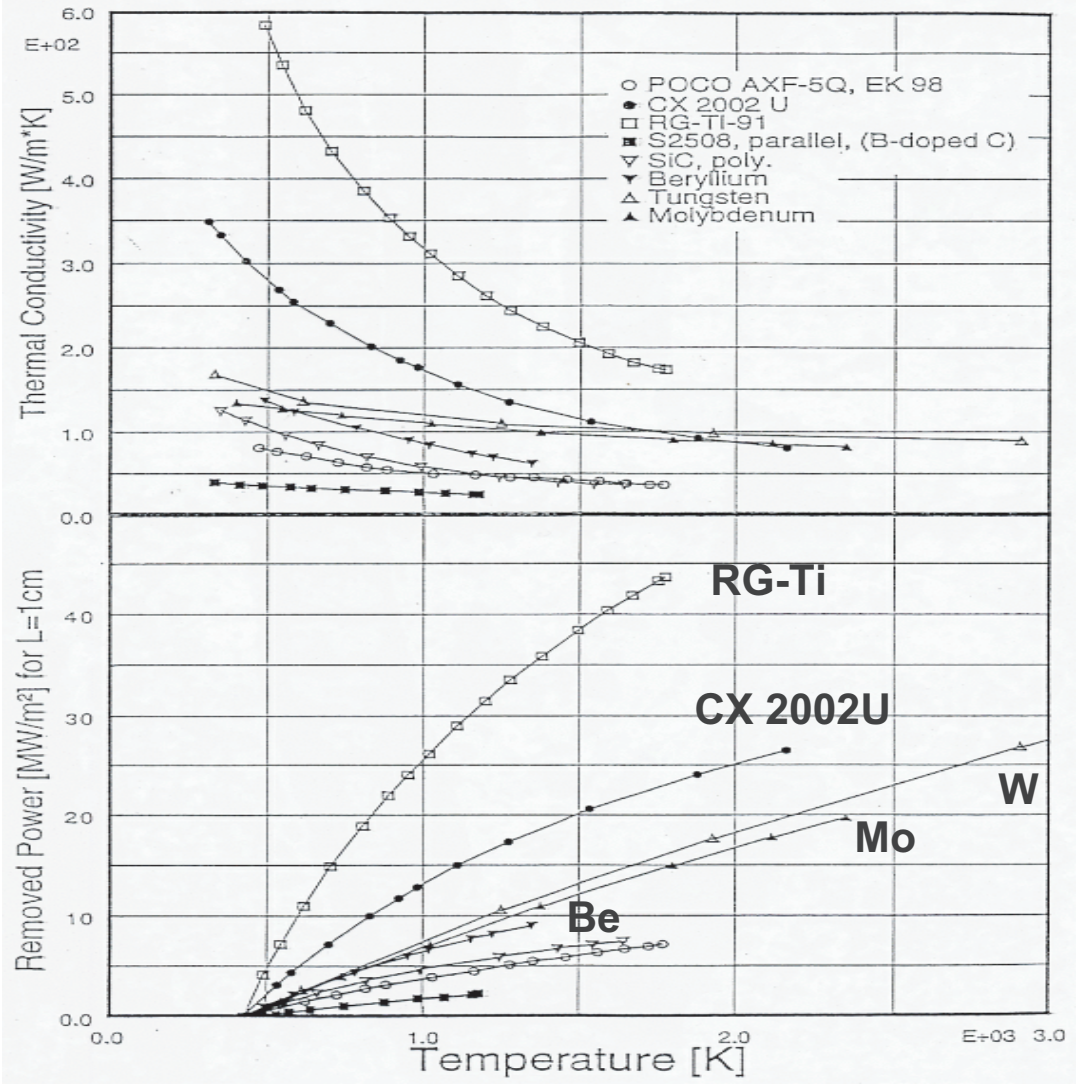
saturation at high fluences, independent of doping





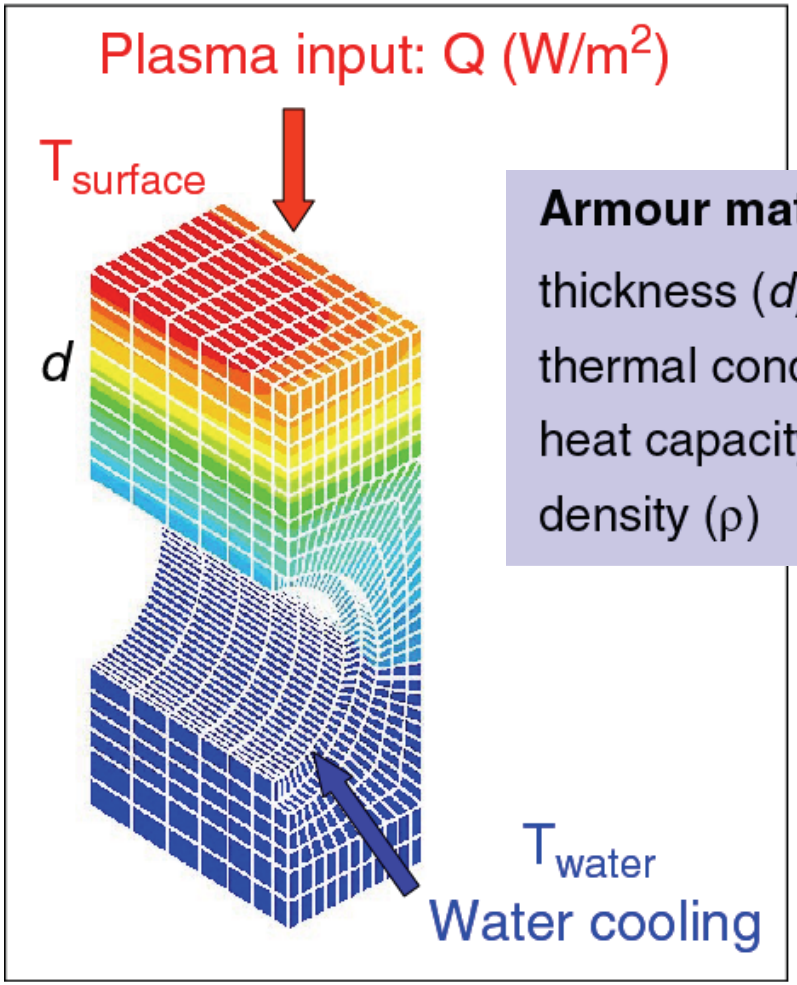
heat load issues

Selection criteria - wall material as heat sink



- specified for heat loads up to10 MW/m^2 in steady state
- higher heat loads in transient events
- only achieved for few materials without melting
- best candidates: graphites, W, Mo

Heat removal - stationary



Armour material

thickness (d)

thermal conductivity (λ)

heat capacity (c)

density (ρ)

Steady state conditions:

$\Delta T = T_{surface} - T_{water} = Q \times d / \lambda$

Typical parameters:

Q =10 MW/m^2, λ = 200W/mK, d = 0.02m, ΔT = 1000 ˚C

PWW issues for Future fusion devices: Loading conditions

	ITER First Wall	ITER Divertor target	Reactor (Demo) First Wall	Reactor (Demo) Divertor target
av. neutron fluence (MW a m^{-2})	0.3	max. 0.15 *	10	5
Normal operation				
No. of cycles	30000	10000 ?	< 1000	< 1000
Peak particle flux (10^{23} $m^{-2}s^{-1}$)	0.01	~10	0.02	~10
Surface heat flux (MW m^{-2})	< 0.5	~10 **	< 1	… 10 …
ELM energy density (MJ m^{-2})	–	< 1	–	reduced
ELM duration (ms) / {Frequency}	–	0.2 / {few Hz}	–	
Off-normal operation				
Peak surface heat load (MJ m^{-2})	60 (VDEs)	30 (Disruptions)	–	?
Duration (ms)	300	1–10	–	1–10, max. 10 events

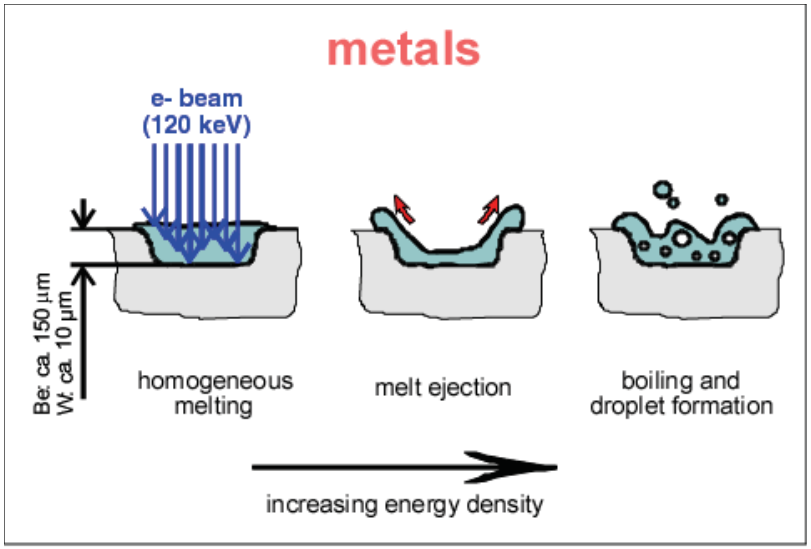
* *without replacement*

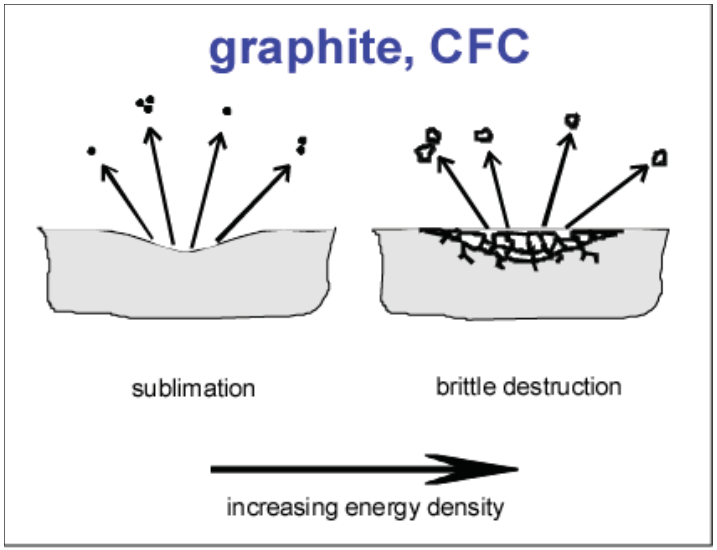
** *slow transients 20 MW m^{-2} lasting 10 s*

Source: H. Bolt et al., J. Nucl. Mater. 307-311 (2002) 43

ELM mitigation is a current research topic: pellet triggering, magnetic perturbation

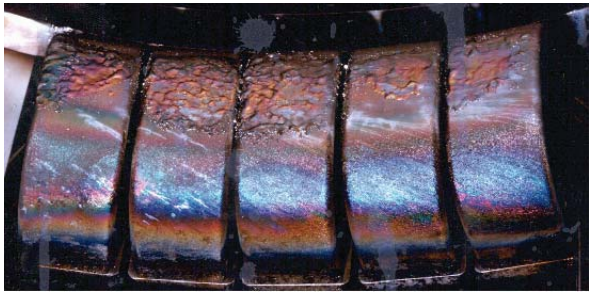
Material erosion under extreme power load

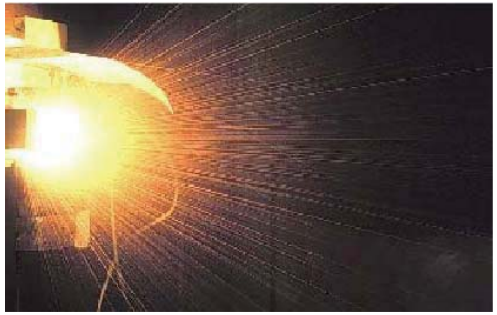




FOR METALS:
Splashing
Formation of droplets
Formation of dust

FOR CARBON:
Above a certain power load (threshold) emission of debris
BRITTLE DESTRUCTION

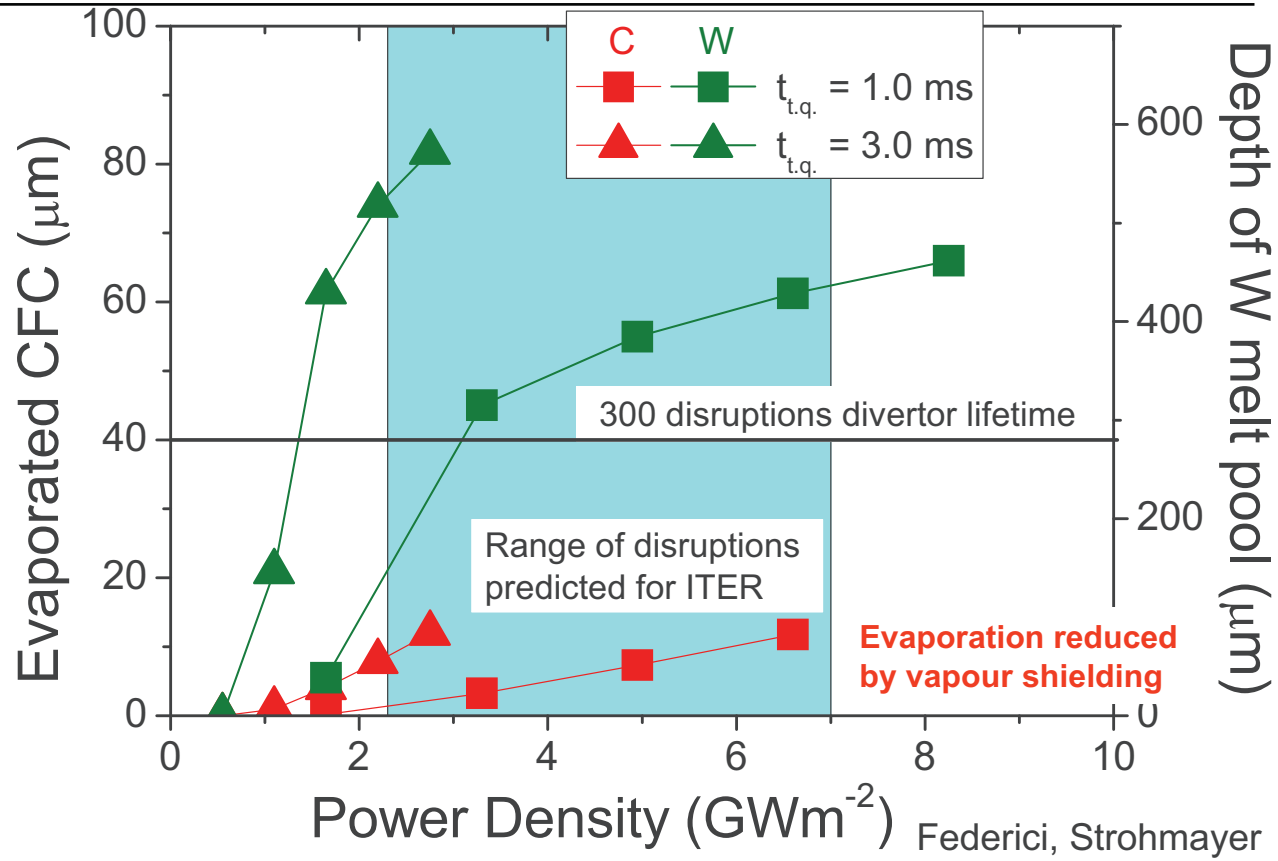




disruption induced erosion:

Lifetime of PFCs

- vapour shielding reduces CFC evaporation by factor 10
- predicted ITER disruptions exceed the 300 disruptions lifetime limit for W
- **efficient mitigation methods needed**



Federici, Strohmayer
RACLETTE
Riccardo, Federici
Nuclear Fusion 2005

ITER assumptions:

30 disruptions in about 2000 discharges

10 % of melt layer lost in the case of W divertor plates

5 kg erosion per disruption

Heat removal - transient

By MHD instabilities (disruptions, edge localised modes - ELMs) a fraction of the plasma stored energy is deposited in short pulses on plasma facing components

Size scaling! ⇒ No problem for present fusion experiments BUT:

Example - ELMs in ITER

$W_{thermal}$	350 MJ
energy drop	2-6 %
per ELM	≈ 15 MJ
deposition time	0.1 - 0.5 ms
deposition area	6 m^2
power density	≈ 10 GW/m^2

Heat removal - transient

In transient events the energy must be absorbed by the target material. Heat capacity is essential (inertial cooling)

$$T(t) = P * (2/\pi\ \lambda\ \rho\ c)^{0.5} * t^{0.5}$$

temperature — power — conductivity — density — heat capacity

$t = 0.00025$ s $\rightarrow$ $T_{max} = 6000\ ^{o}C$ **Penetration depth: 0.15 mm**

$Graphite_{subl.\ thresh.}$ = 2200 °C *Tungsten: T_m = 3410 °C, T_b = 5660 °C*

Graphite target will sublimate quickly and undergo brittle destruction

Metals will melt $\Rightarrow$ loss of melt layer by forces on induced currents

No material solution $\Rightarrow$ Plasma physics must solve this problem!

What suitable materials are left?

HIGH THERMAL CONDUCTIVITY	CFC-Cu alloy + W-Cu alloy
GOOD THERMO - MECHANICAL PROPERTIES (RESPONSE TO THERMAL SHOCKS)	CFC
LOW NEUTRON ACTIVATION (NEUTRON FLUX $> 10^{17}$ m^{-2} s^{-1})	Be + CFC V-Ti + SiC (structure)
RESISTANCE TO RADIATION DAMAGE (TO AVOID SWELLING AND EMBRITTLEMENT)	CFC
LOW CHEMICAL AFFINITY TO HYDROGEN (NO FORMATION OF VOLATILE COMPOUNDS)	Be + W
LOW ACCUMULATION OF HYDROGEN (TRITIUM INVENTORY MUST NOT EXCEED 0.35 kg)	W + Be (?)
REACTIVITY WITH OXYGEN TOWARDS THE FORMATION OF STABLE AND NON-VOLATILE OXIDES (GETTERING OF OXYGEN IMPURITIES)	Be

Exercises

1) Calculate first wall or divertor plate erosion based on chemical sputtering
For example, assume the following conditions:

	T_{surf}(K)	E_0 (eV)	flux Γ ($m^{-2}s^{-1}$)
Divertor	700	30	10^{23}
First wall	500	200	10^{20}

Comparison can be made with physical sputtering to see which process dominates under which conditions. What might be the implication of having an all-carbon ITER?

2) Try to describe schematically the depth distribution of D in a 500 μm W foil

- for the case of purely diffusion limited release. What would be the ratio of the re-emitted flux to the permeating flux in steady state assuming an ion range of 50 nm.
- for the case of strongly recombination limited surface facing the plasma.
- What would be the optimum position of a diffusion barrier to limit the T inventory inside the first wall