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- **Chemical sputtering**
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- **Impact of impurities on fusion plasmas**

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# Introduction

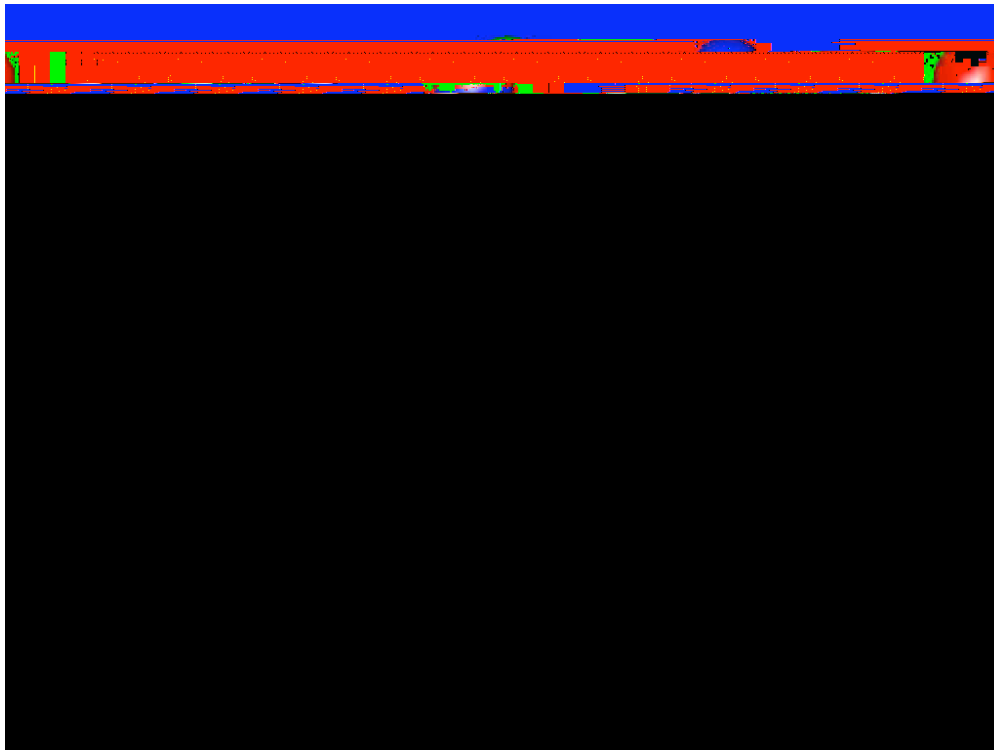
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Molecular Dynamics simulation of 50eV He Be



Energetic particle impact involves a complex collision cascade during which:

!The projectile may be reflected back out of the surface

!The projectile may remain in the surface (=implantation)

Surface atoms may be ejected out from the surface (= physical sputtering)

!The surface may be left with crystal damage.

Energetic particle impact is a stochastic process and is therefore described by giving average yields for the different processes

- Physical sputtering is the kinetic ejection of surface atoms by incident energetic ions or atoms due to collision processes.
- As surface atoms can escape only if it receives an energy larger than the surface binding energy, a threshold energy for the incident particles is required.
- In fusion application physical sputtering by hydrogen ions and atoms is important, but also the self-sputtering due to returning impurity atoms.

- TRIM Monte-Carlo Code simulation

### **Heavy ions:**

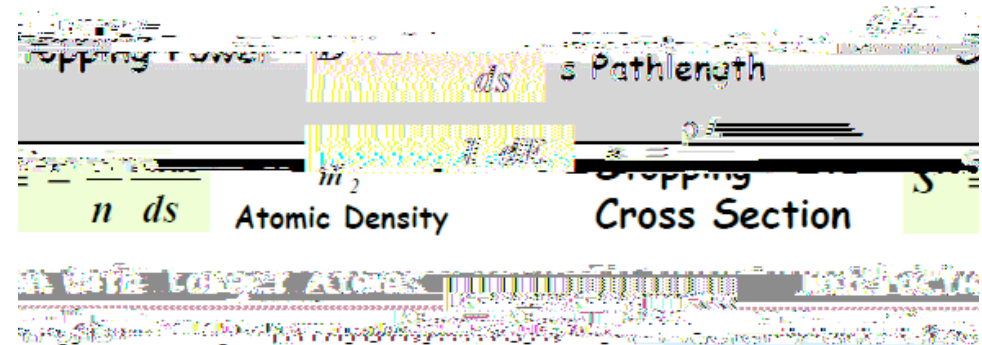
- large collision cascade
- isotropic velocity distribution
- yield proportional to energy deposited in first 0004fy



# Physical sputtering



stopping power



Stopping power is velocity dependent

Fast particles stopping dominated by  $S_e$

Slow particles stopping dominated by  $S_n$



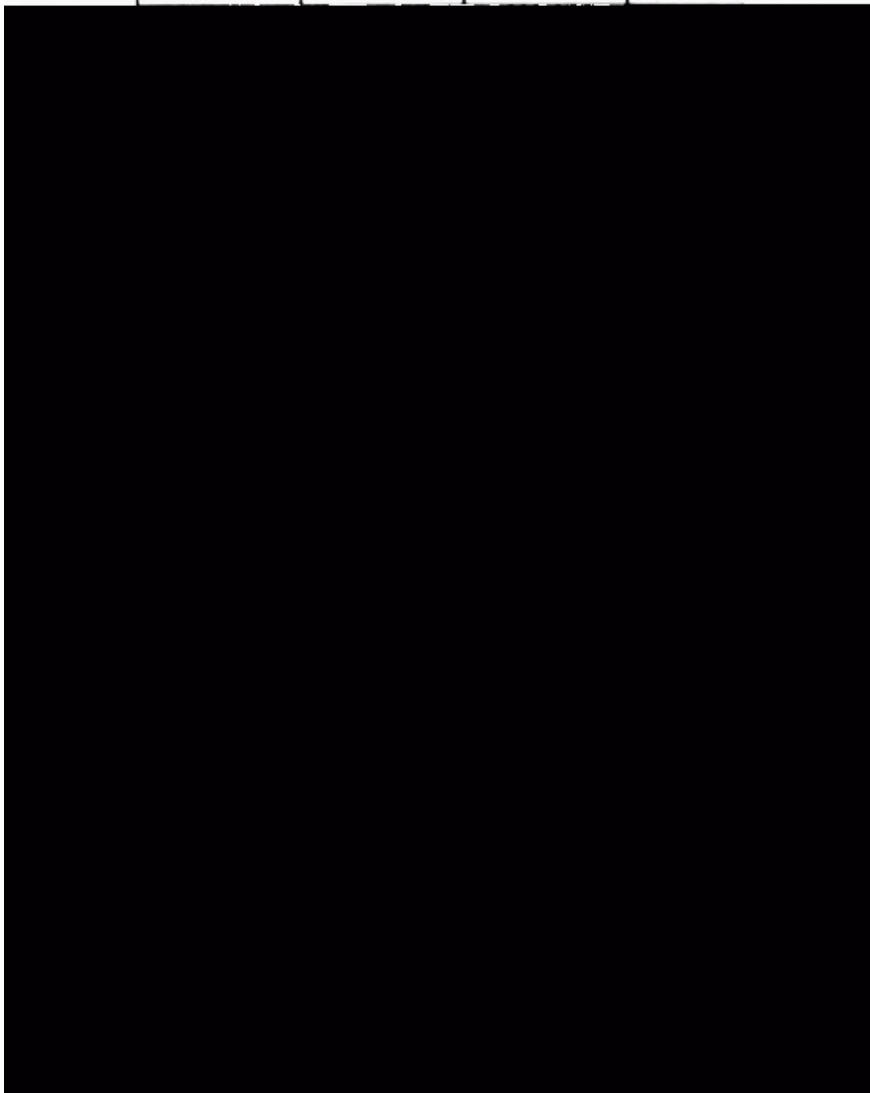


## Threshold energy



- Light ion sputtering in fusion application is dominated by threshold effects

## Theory for sputtering in isotropic collision cascades



Ansatz:

(P. Sigmund (1969))

Sputtering yield proportional to the energy deposited into collisions near the surface

$$Y(\ ) = S_n(\ )_{x=0} / E_s$$

$$Y(\ ) = Q(M_1, M_2, E_s) * f_H(\ )$$

$E_s$  = Surface binding energy      H  
heat of sublimation

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## physical sputtering

- Physical sputtering is the ***kinetic ejection of surface atoms*** by incident energetic ions or atoms ***due to collision processes*** (playing pool with surface atoms).
- As surface atoms can escape only if it receives an energy larger than the ***surface binding energy***, a threshold energy for the incident particles is required.
- In fusion application sputtering by hydrogen and helium ions and atoms is important, but also the self-sputtering due to returning impurity atoms.

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# Chemical Erosion

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- Chemical erosion originates from the formation and release of volatile molecules in the interaction of incident plasma particles and target atoms.
- In fusion application the formation of hydrocarbons in the interaction of hydrogen atoms with carbon surfaces is the dominant example of chemical erosion
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$sp^2$

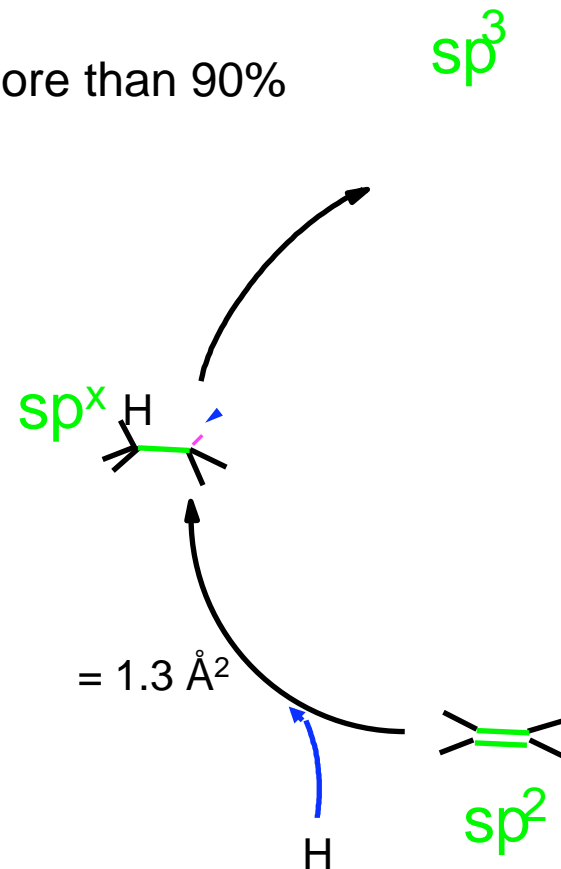
# chemical erosion: microscopic model

## Hydration and erosion circle:

Horn et al., Chem. Phys. Lett. 231, 193 (1994)

Zecho et al. J. Phys. Chem. B 105 (2001).

- hydration at room temperature of more than 90% of all possible adsorption sites
- erosion maximum as function of temperature







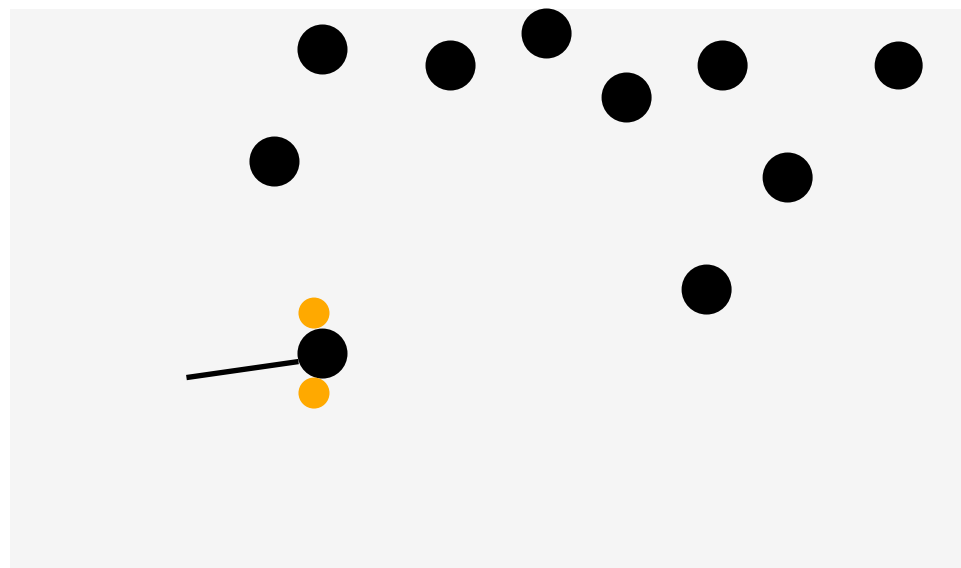
## chemical erosion

- chemical erosion originates from the formation and release of volatile molecules in the interaction of incident plasma particles and target atoms.
- in fusion application the formation of hydrocarbons in the interaction of hydrogen atoms with carbon surfaces is the dominant example of chemical erosion.
- as chemical reactions are involved, chemical erosion shows a strong temperature dependence in contrast to physical sputtering.
- chemical erosion can occur with low-energy ions or thermal atoms and does not require a threshold energy.
- erosion will only take place at the very surface (1.4 nm penetration depth) or at the end of range of energetic particles.



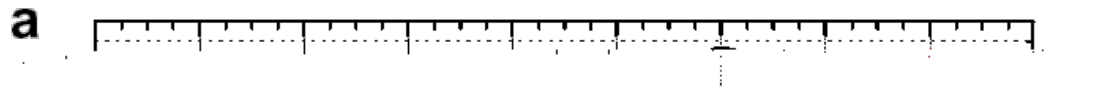
*it is not chemical erosion*

H<sup>0</sup> at  $T > 400$  K with a max. at





## Temperature dependence



- Temperature dependence similar as for chemical erosion
- Radiation damage enhances chemical reactivity
- Value at  $T_{\max}$  is larger than sum of chemical erosion and low temperature chemical sputtering



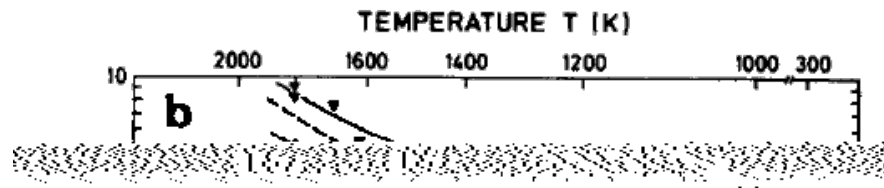




# Radiation enhanced sublimation



Exponential fits yield activation energies



- Arrhenius activation energies are well below the graphite sublimation energy.
- Process occurs for both inert and reactive sputtering species
- Experiments indicate that eroded species have thermal energies



- Diffusion trapping model quantitatively describes RES

- Damage profile calculated by TRIM.

- Under fusion conditions the influence of RES is not very pronounced:

At high fluxes the vacancy concentration becomes very high leading to fast annihilation of the more mobile interstitials.

For low particle energies close to the damage threshold no Frenkel pairs are created.

- At high temperatures graphite exhibits an exponential increase in the erosion rate during energetic particle impact that can not be explained by sublimation
- A model using the sublimation of weakly bonded surface defects, quantitatively describe the process.
- Similar effects are also seen for metallic targets at very high fluxes and temperatures. more relevant for fusion.

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# Impact of impurities on fusion plasmas

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- As atoms are eroded from the first wall they enter the plasma
- In the plasma they are ionized and transported throughout the machine.
- What how does that affect the plasma ?

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# Impact of impurities on fusion plasmas

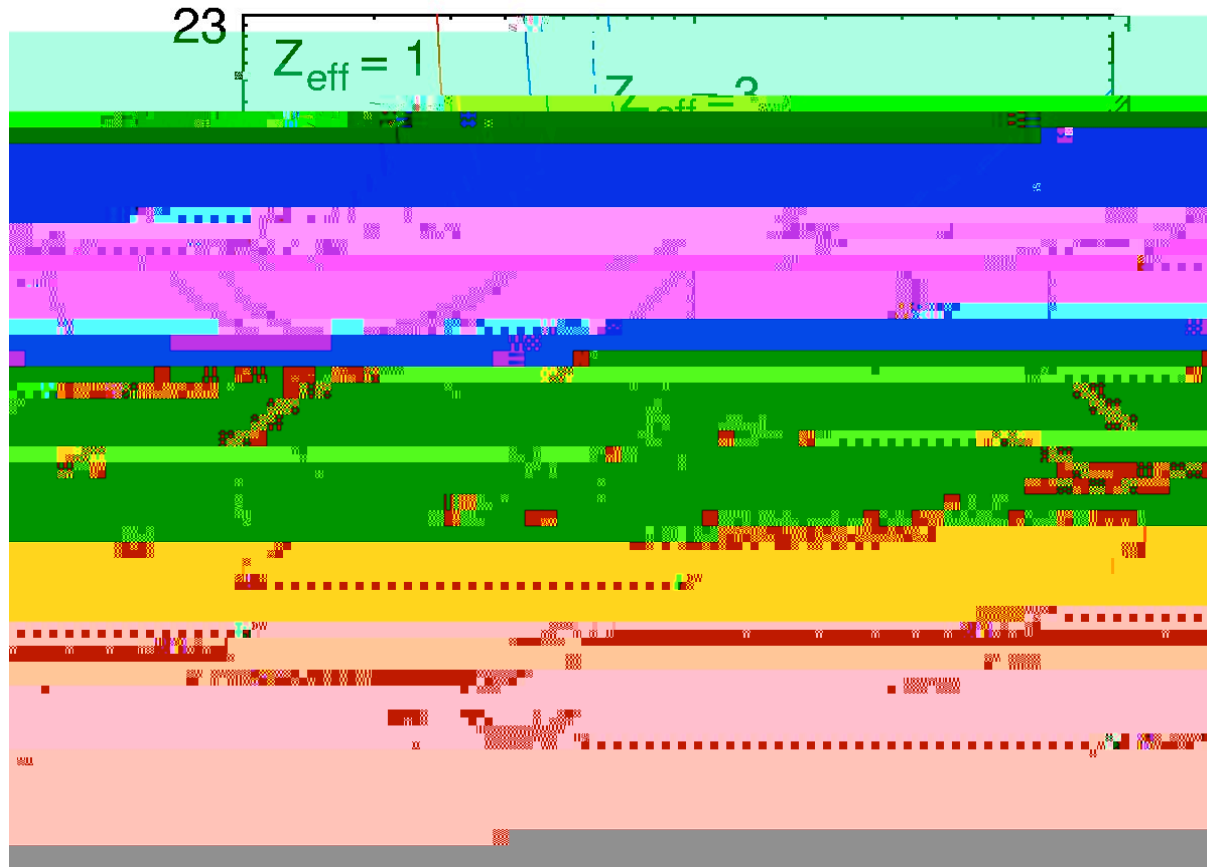
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# Impact of impurities on fusion plasmas

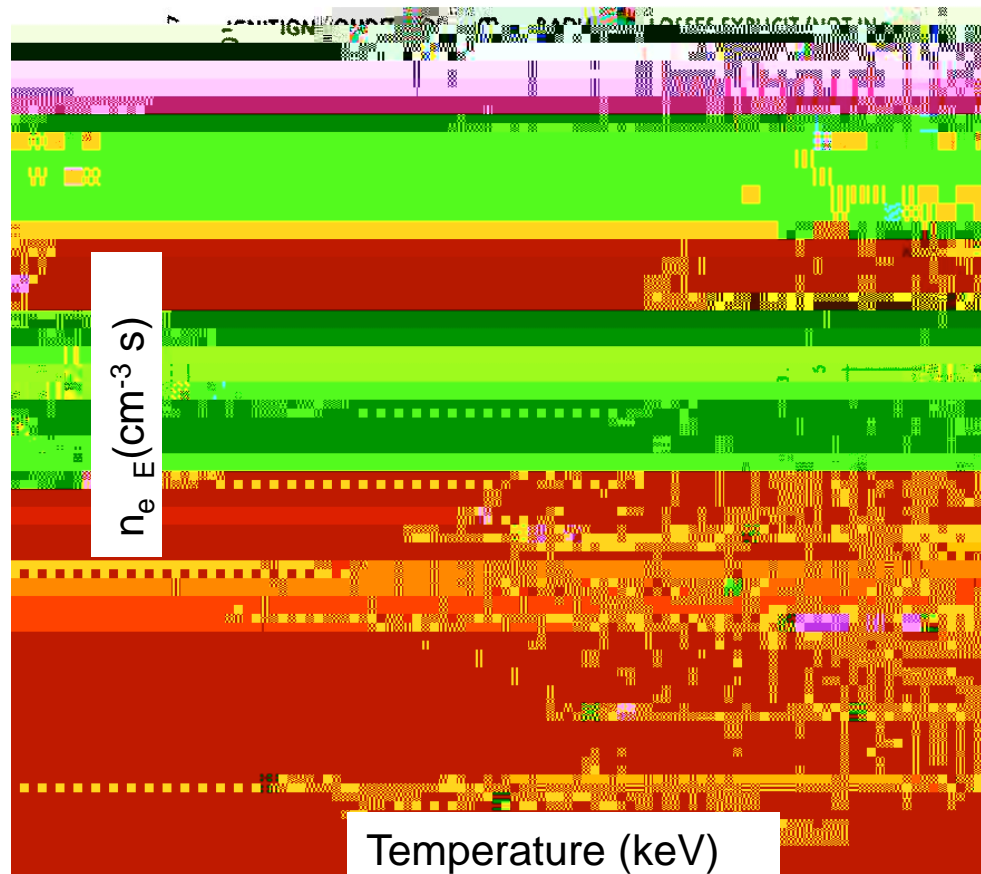
## Ignition Criteria

- **Ignition:** The neutrons leave the plasma, the  $\alpha$ -particles are confined and heat it. Only their energy should enter the balance!  $E_{\text{fus}} = E$





- The  $\alpha$ -particles also dilute the plasma, as they are intrinsically coupled to fusion power ( $3.53 \cdot 10$ )

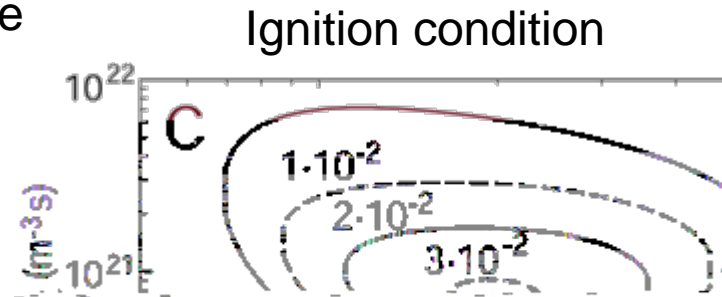


# Impact of impurities on fusion plasmas



- Other impurities have a similar impact as He

- Dilution of fuel ions



...  $P_R$

! No ignition for core W conc.  $> 10^{-4}$

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- As atoms are eroded from the first wall they enter the plasma
- In the plasma they are ionized and transported throughout the machine.
- In the plasma they radiate energy through line radiation and Bremsstrahlung.
- They also dilute the plasma.
- The radiative loss of energy from the plasma and its dilution through these impurities has fundamental implications for the operation of a fusion reactor!
- The erosion of wall components poses a lifetime problem
- The co-deposition of impurities (mainly C) with fuel ions poses a radiation hazard