Max-Planck-Institut
für Plasmaphysik

BRIDGING THE GAP BETWEEN PWI DATA AND FUSION EXPERIMENTS

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- How does PWI influence the fusion plasma

Linking impurity migration and surface evolution
- The WallDYN concept
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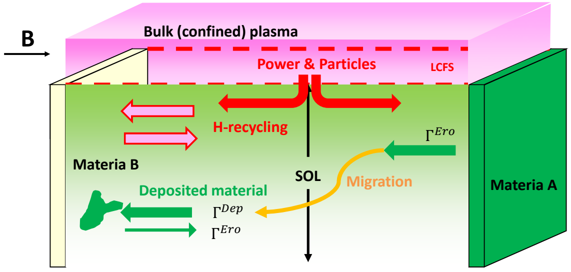
- Fill level dependent trapping: From DFT to lab experiments
- Example: Isotope exchange at ambient temperatures

Summary

Introduction

How does PWI influence the fusion plasma

❖ **Principle picture**



❖ H (D, T) recycling (implantation & (out-diffusion)) determines the neutral particle dynamics in the SOL

❖ Erosion produces plasma impurities that migrate and re-deposit

❖ Deposition and re-erosion changes impurity source distribution

→ Tight coupling between plasma and surface processes

→ **Need to include plasma to predict surface evolution**

Introduction

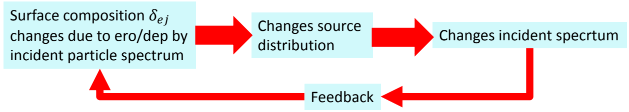
How does PWI influence the fusion plasma

❖ **What drives surface evolution**

❖ Erosion flux of element „ei“ $\Gamma_{ei}^{Ero} \propto$
- Partial erosion yield $Y_{ei\ by\ es}^{Part}$
- Incident particle spectrum $\Gamma_{es}^{In}(E)$ species „es“ at energy „E“

❖ Deposition flux of element „ei“ $\Gamma_{ei}^{Dep} \propto$
- Reflection yield R_{ei}
- Incident flux of ei $\Gamma_{ei}^{In}(E)$

❑ $Y_{ei\ by\ es}^{Part} \propto$ Surface composition δ_{ej} of all elements
❑ $R_{ei} \propto$ Surface composition δ_{ej} of all elements
❑ $\Gamma_{es}^{In}(E) \propto$ Source distribution (i.e. δ_{ej} on different wall elements) and plasma transport



Surface composition δ_{ej} changes due to ero/dep by incident particle spectrum

Changes source distribution

Changes incident spectrum

Feedback

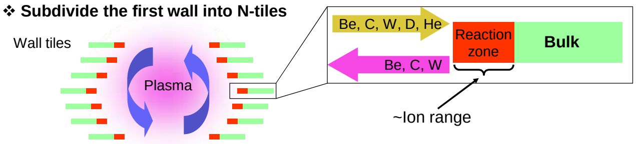
Linking impurity migration and surface evolution

The WallDYN concept

Linking impurity migration and surface evolution

The WallDYN concept

❖ **Subdivide the first wall into N-tiles**



❖**Plasma model [1]:**
- Plasma transport can be characterized by a re-deposition matrix:

$$r_{wj,wk}^{ei,qi} \equiv \text{Fraction of eroded flux of element ei at charge state qi from wall tile wj that ends up on tile wk}$$

❖**Surface model[1,2]:**
- All erosion & deposition is assumed to occur homogeneously in the reaction zone:

$$\frac{d\delta_{ei,wr}}{dt} \equiv \text{Areal density time evolution of element ei on wall wr} = \text{Incident flux} * (1 - \text{Reflection}) - \text{Eroded Flux} + \text{Bulk exchange}$$

[1] K. Schmid et al J. Nucl. Mat 415 (2011) S284–S288
[2] K. Schmid et al., Nuclear Technology, 159, No. 3, (2007) 238

Linking impurity migration and surface evolution

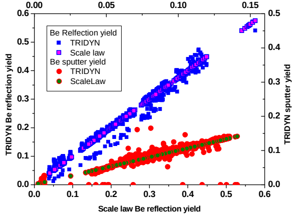
The WallDYN concept

- **Main features**
  - **Non iterative** merge of **global impurity transport** (DIVIMP) with **surface models** (Sputtering, Chemical erosion, Sublimation, Seeding...)
  - Includes **re-erosion** of deposited material
  - Maintains a strict **global material balance**
- **Implementation**
  - Use continuous description of surface and plasma flux evolution using ODE's and AE's
  - Yields a DAE system that allows to **truly couple** different physical processes
  - Solved using an implicit BDF solver
- **Advantage over iteratively coupling MC, MD or DFT codes**
  - Iterative coupling occurs on different time scales
  - Error propagation during iterative coupling
  - Sampling artefacts in MC-based codes
  - Last but not least: Computation time

Linking impurity migration and surface evolution

The WallDYN concept

- Input into the WallDYN **surface model:**
  - Mixed material sputter yields $Y_{ei\ by\ ej}\left(\langle\ \delta_{ek}\rangle, E_{ej}, \alpha, T\right)$
    - ☐ Depends on all elements in the mixture, Energy, angle and temperature
    - ☐ Taken from SDTRIM.SP parameter scans, Experiment, MD....
  - Reflection yield of projectiles from mixed materials $R_{ei}\ (\langle\ \delta_{ek}\rangle, E_{ei}, \alpha)$
    - ☐ Depends on all elements in the mixture, Energy, angle
    - ☐ Taken from dynamic TRIM, Experiment, MD....
- WallDYN is a non iterative contineous code
  → Analytic expression required
  → Fit scaling laws to reflection and sputter yield data
- Example Be data for a Be, C, W mixture
  - Reasonable fit to database



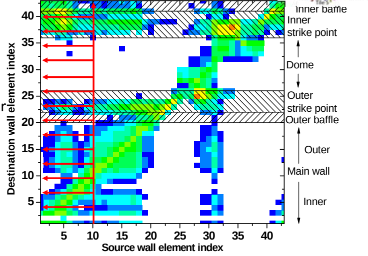
Linking impurity migration and surface evolution

The WallDYN concept

- Input into the WallDYN **plasma migration model**:
  - Redistribution matrix

    $r_{wj,wk}^{ei,qi} \equiv$ Fraction of eroded flux of element ei at charge state qi from wall tile wj that ends up on tile wk
  - Calculated by trace impurity code DIVIMP
- **Example** charge state integrated Be redistribution matrix
  - Diagonal points towards strong local re-dep
  - Plasma flows point towards inner divertor
    → Strong deposition on Baffles

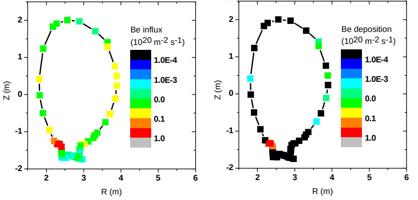
$r_{i,j}^{Be}$ Be, redistribution matrix

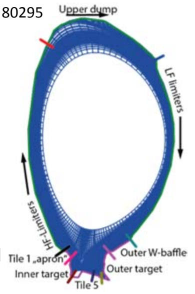


Linking impurity migration and surface evolution

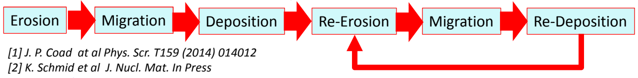
Example: Be migration in JET-ILW [2]

- Be influx and deposition during L-Mode divertor phase JET-ILW 80295





- WallDYN calculates evolution of Be influx and Be deposition
- Be deposition pattern in excellent agreement with literature [1]
- **Be influx does not mean deposition**
  - ☐ Erosion source strength + plasma transport are not enough to predict deposition
  - ☐ Need to include the entire transport chain:

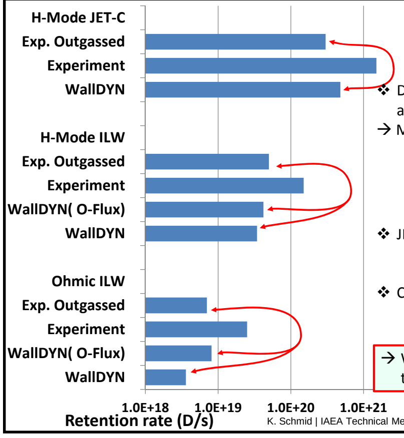


Erosion → Migration → Deposition → Re-Erosion → Migration → Re-Deposition

[1] J. P. Coad at al Phys. Scr. T159 (2014) 014012
[2] K. Schmid et al J. Nucl. Mat. In Press
doi:10.1016/j.jnucmat.2014.11.109

Linking impurity migration and surface evolution

Example: Be migration in JET-ILW



Experimental data from:
S. Brezinsek et Al Nucl. Fusion 53(2013) 083023

- D/X ratios based on post mortem analysis
  → Must include long term outgassing
  - JET-ILW:
    Outgassing was measured
  - C-JET:
    Gas balance/post mortem = 1/5
- JET-ILW:
  - D/Be at tile 1 „Apron" 1 to 4%
  - D/Be in remote areas 40%
- C-JET:
  - D/C ~40% at base temp.
  - D/C ~ 5% at high temp.

→ WallDYN matches experiment if long term ougassing is taken into account

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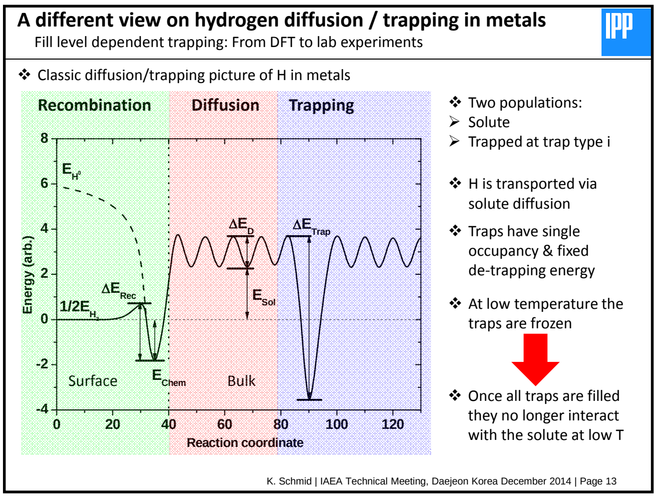
A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments



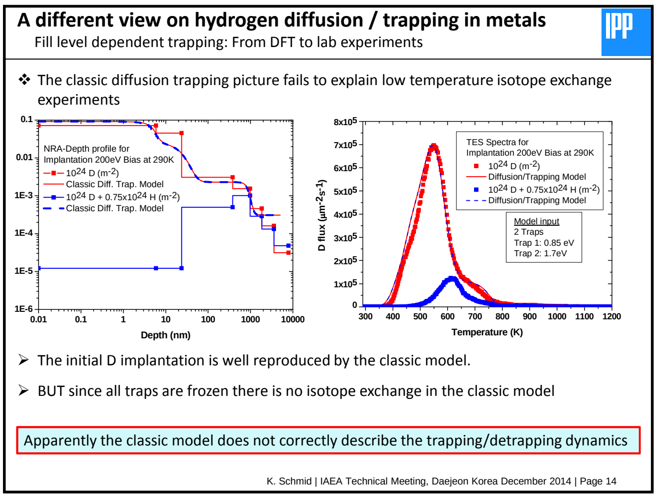
A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments

- Classic diffusion/trapping picture of H in metals

- Two populations:
  - Solute
  - Trapped at trap type i
- H is transported via solute diffusion
- Traps have single occupancy & fixed de-trapping energy
- At low temperature the traps are frozen

- Once all traps are filled they no longer interact with the solute at low T



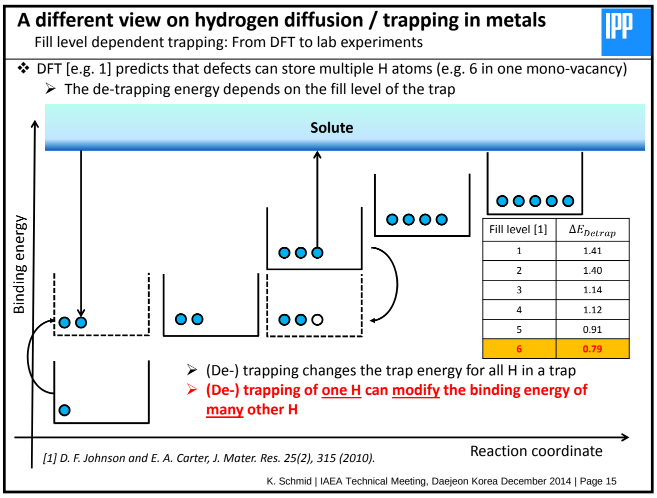
A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments

- The classic diffusion trapping picture fails to explain low temperature isotope exchange experiments

- The initial D implantation is well reproduced by the classic model.
- BUT since all traps are frozen there is no isotope exchange in the classic model

Apparently the classic model does not correctly describe the trapping/detrapping dynamics



A different view on hydrogen diffusion / trapping in metals

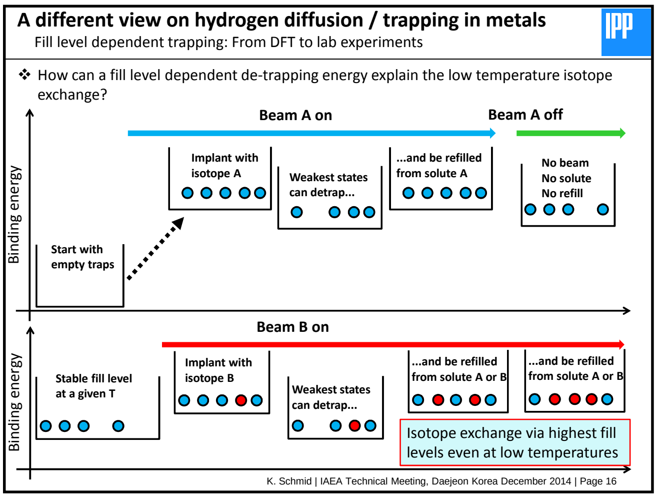
Fill level dependent trapping: From DFT to lab experiments

- DFT [e.g. 1] predicts that defects can store multiple H atoms (e.g. 6 in one mono-vacancy)
  - The de-trapping energy depends on the fill level of the trap

Fill level [1]	ΔE_{Detrap}
1	1.41
2	1.40
3	1.14
4	1.12
5	0.91
6	0.79

- (De-) trapping changes the trap energy for all H in a trap
- **(De-) trapping of one H can modify the binding energy of many other H**

[1] D. F. Johnson and E. A. Carter, J. Mater. Res. 25(2), 315 (2010).

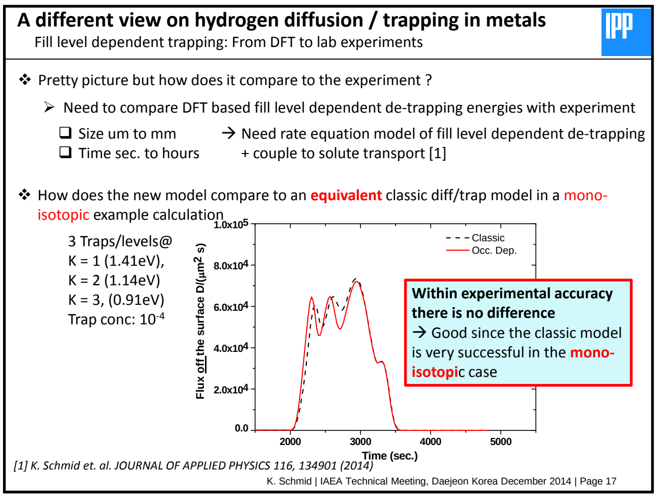


A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments

- How can a fill level dependent de-trapping energy explain the low temperature isotope exchange?

Isotope exchange via highest fill levels even at low temperatures



A different view on hydrogen diffusion / trapping in metals

Fill level dependent trapping: From DFT to lab experiments

- Pretty picture but how does it compare to the experiment ?
  - Need to compare DFT based fill level dependent de-trapping energies with experiment

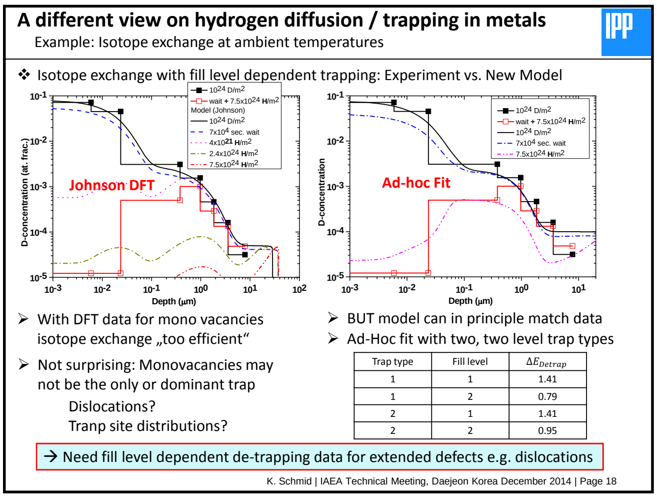
☐ Size um to mm → Need rate equation model of fill level dependent de-trapping
☐ Time sec. to hours + couple to solute transport [1]

- How does the new model compare to an **equivalent** classic diff/trap model in a mono-isotopic example calculation

3 Traps/levels@
K = 1 (1.41eV),
K = 2 (1.14eV)
K = 3, (0.91eV)
Trap conc: 10^{-4}

Within experimental accuracy there is no difference
→ Good since the classic model is very successful in the **mono-isotopic** case

[1] K. Schmid et. al. JOURNAL OF APPLIED PHYSICS 116, 134901 (2014)



A different view on hydrogen diffusion / trapping in metals

Example: Isotope exchange at ambient temperatures

- Isotope exchange with fill level dependent trapping: Experiment vs. New Model

- With DFT data for mono vacancies isotope exchange „too efficient“
- Not surprising: Monovacancies may not be the only or dominant trap

  Dislocations?
  Tranp site distributions?

- BUT model can in principle match data
- Ad-Hoc fit with two, two level trap types

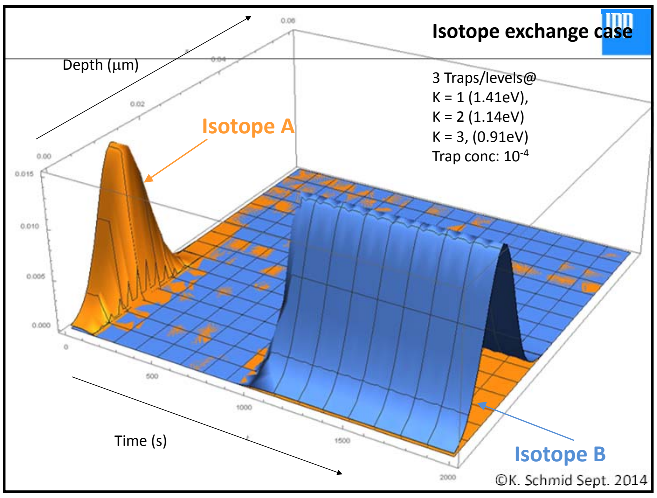
Trap type	Fill level	ΔE_{Detrap}
1	1	1.41
1	2	0.79
2	1	1.41
2	2	0.95

→ Need fill level dependent de-trapping data for extended defects e.g. dislocations

Summary

- ❖ WallDYN allows to couple surface process data from different source to plasma transport
- ❖ WallDYN calculates global impurity migration, erosion, layer deposition and co-deposition
- ❖ WallDYN tracks the entire erosion/migration/deposition/re-erosion chain
  - ➢ **Main input: mixed material sputter and reflection yields**
  - ➢ **Currently taken from dynamic TRIM (calculations)**

- ❖ The classic Diff./Trapp. model does not correctly describe the trapping/detrapping dynamics
- ❖ DFT predicted fill level dependence can explain low temperature isotope exchange
- ❖ New rate equation model allows to test DFT predictions against experimental data
- ❖ Classic Diff./Trapp & fill level dependent model indiscernable in mono-isotopic case
  - ➢ **Main input: fill level dependent detrapping energies**
  - ➢ **Currently only available for monovacancies from DFT**
  - ➢ **Maybe use MD for extended defects ?**



Isotope exchange case

3 Traps/levels@
K = 1 (1.41eV),
K = 2 (1.14eV)
K = 3, (0.91eV)
Trap conc: 10^{-4}

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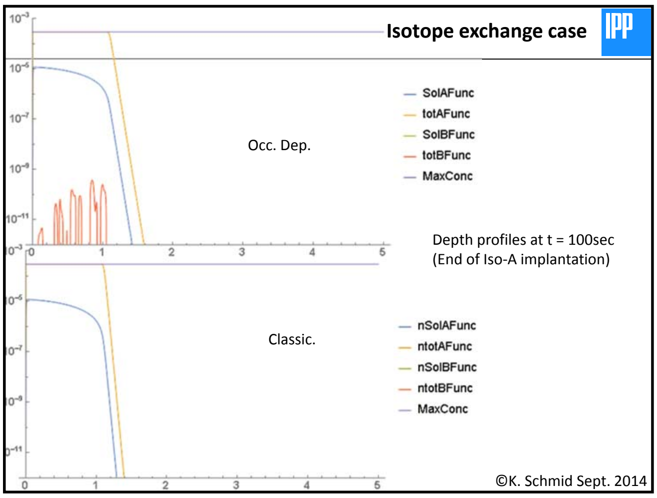
Discussion slides



Isotope exchange case

Depth profiles at t = 100sec
(End of Iso-A implantation)

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Isotope exchange case
T = const = 300K

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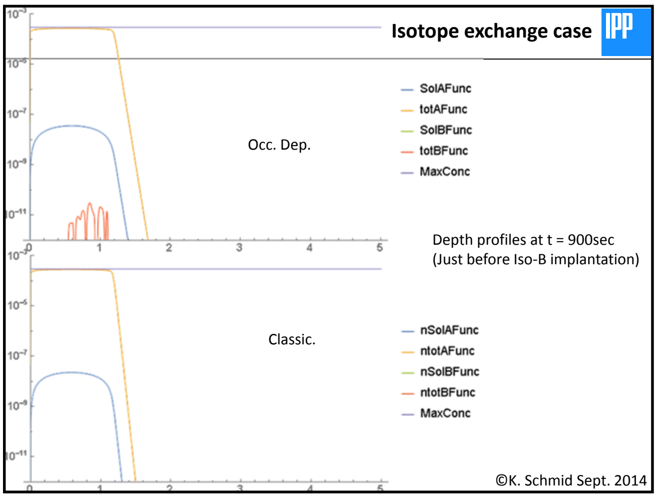

Isotope exchange case

Depth profiles at t = 900sec
(Just before Iso-B implantation)

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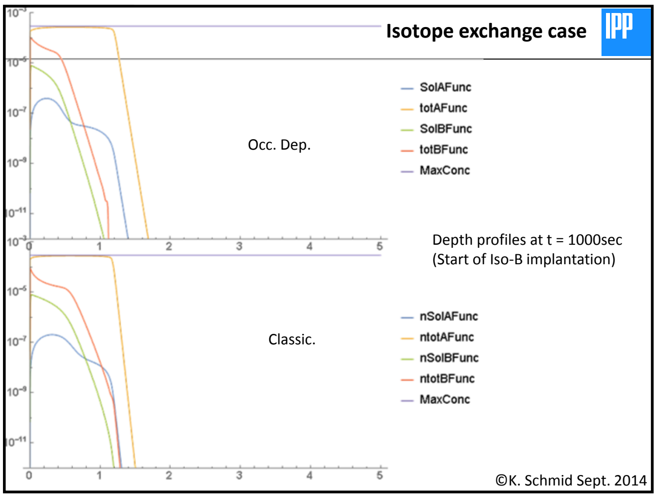
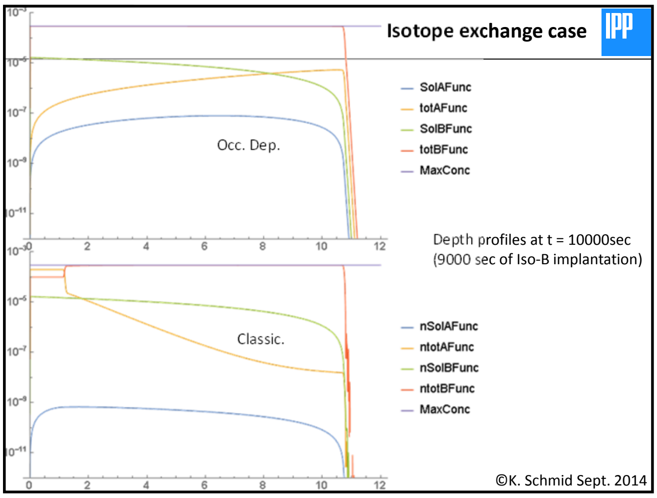


Isotope exchange case

Occ. Dep.

Classic.

Depth profiles at t = 1000sec
(Start of Iso-B implantation)

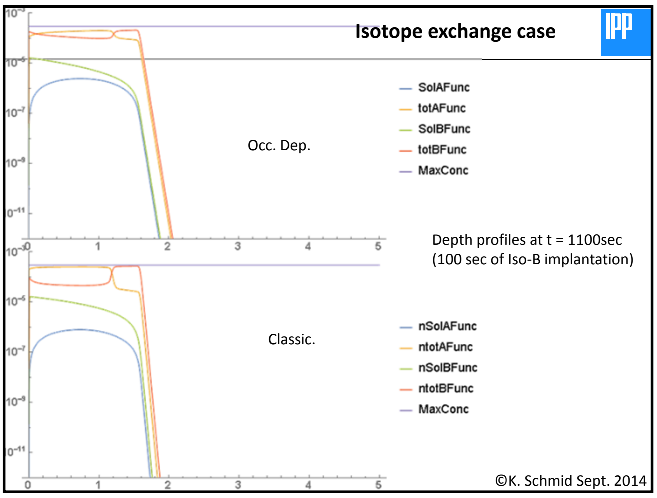


Isotope exchange case

Occ. Dep.

Classic.

Depth profiles at t = 10000sec
(9000 sec of Iso-B implantation)

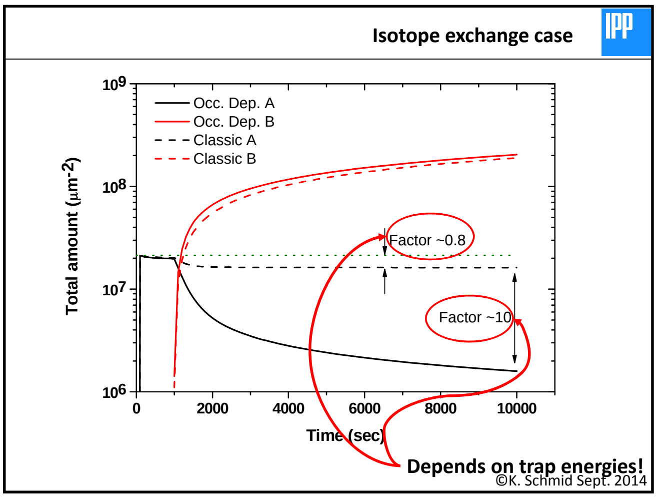


Isotope exchange case

Occ. Dep.

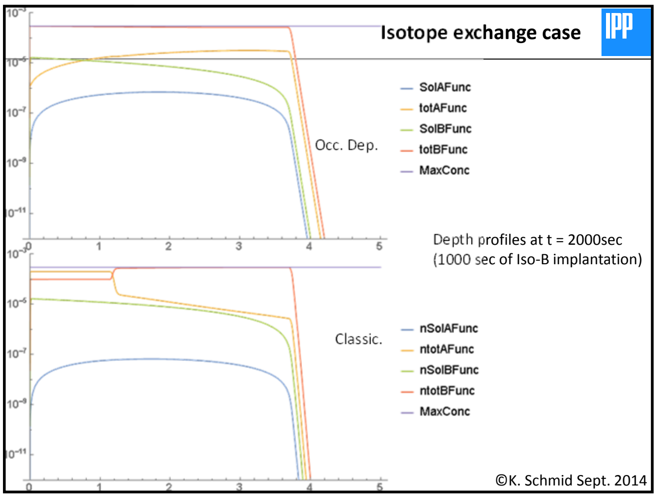
Classic.

Depth profiles at t = 1100sec
(100 sec of Iso-B implantation)



Isotope exchange case

Depends on trap energies!



Isotope exchange case

Occ. Dep.

Classic.

Depth profiles at t = 2000sec
(1000 sec of Iso-B implantation)