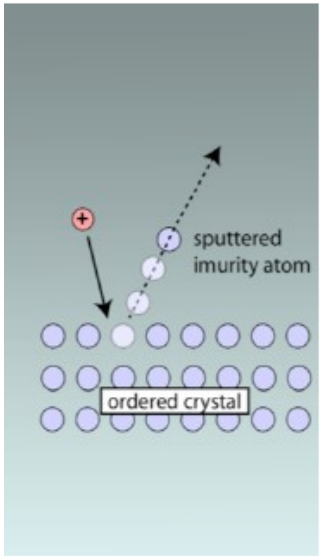
Key parameters for Plasma-Material Interaction

U. von Toussaint, A. Mutzke, D. Coster,
Th. Schwarz-Selinger, R. Preuss

Introduction

Classical Focus of Particle-wall interaction in fusion:

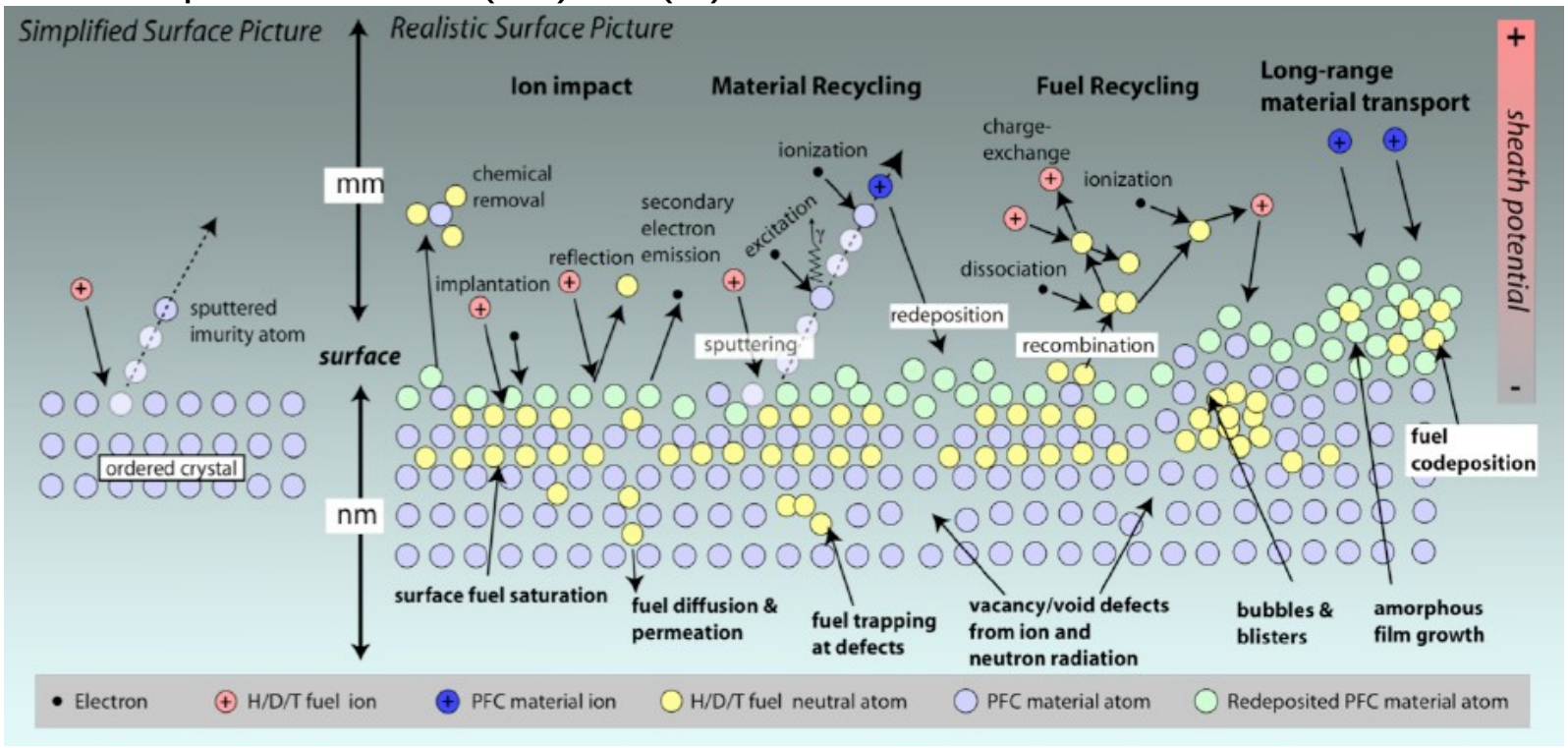
- Sputter yield Y(E,angle,species) and reflection: well studied for pure samples & atomic projectiles
- Collision cascade in binary collision approximation: O(10^{-12} sec)



Introduction

Particle-wall interaction:

- Wall is part of complex PMI interplay
- Time scales O(10^{-12} sec) – O(10^{+3} sec)
- Similar for spatial scales O(nm) – O(m)



by D. Whyte, FPAM (2010)

Large number of coupled processes (→ this meeting).

- Here: hydrogen transport in material

I. Hydrogen transport in materials

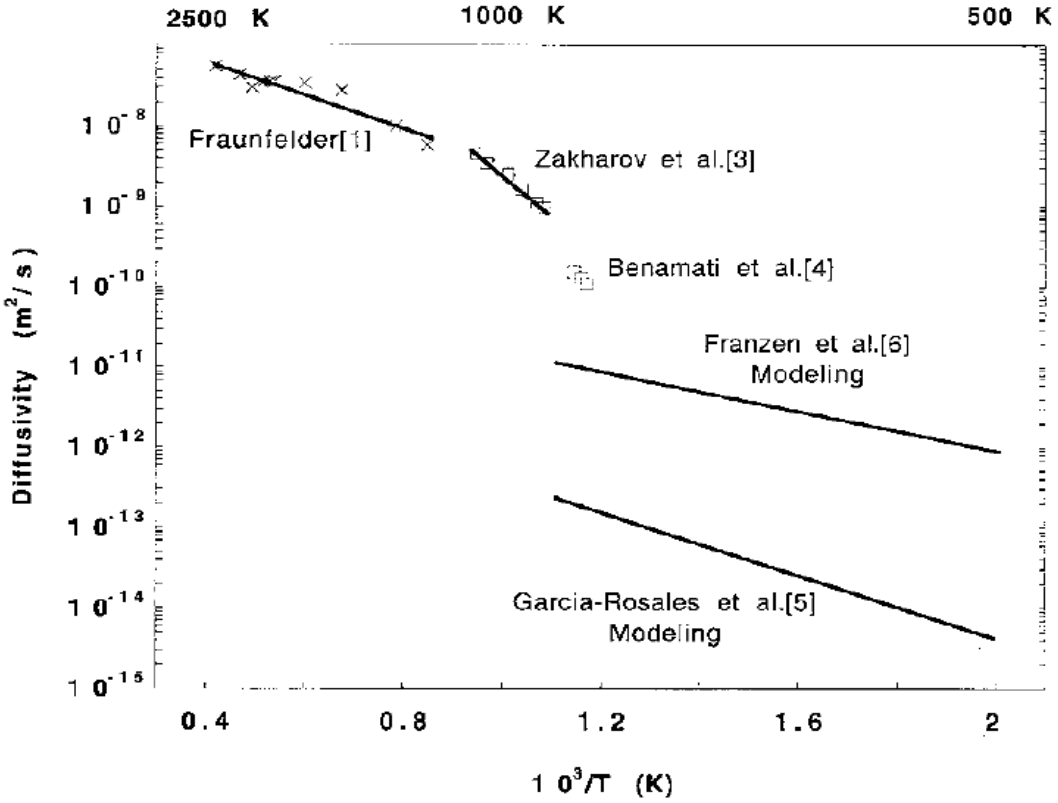
Tritium retention and transport in material crucial

- Key parameters: Diffusion, Solubility, Permeation
- Example: Situation for H in tungsten

I. Hydrogen transport in materials

Tritium retention and transport in material crucial

- Key parameters: **Diffusion**, Solubility, Permeation
- Example: Situation for H in tungsten
- Recommended value: **0.39 eV** (Frauenfelder) [Causey, PhysScr T94,9 (2001)]

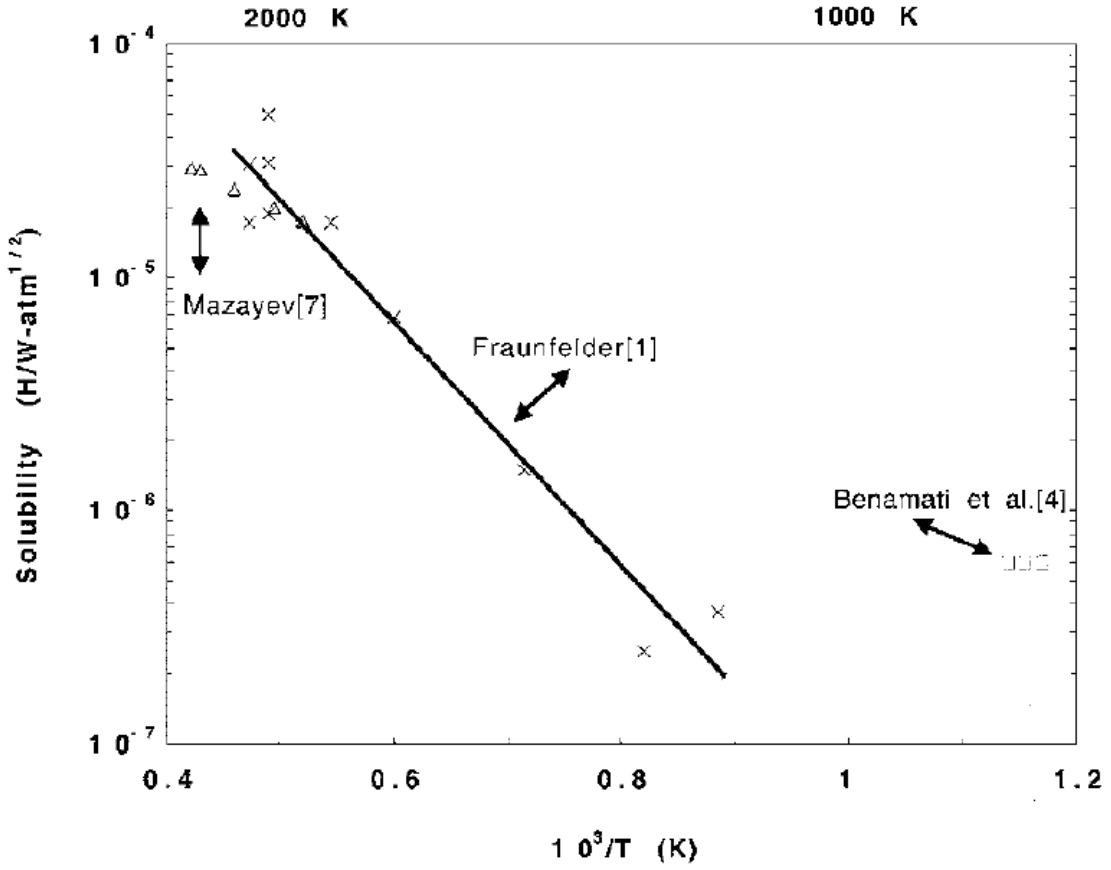


Data from 1969, recent DFT-calculations: **0.25 eV**

I. Hydrogen transport in materials

Tritium retention and transport in material crucial

- Key parameters: Diffusion, **Solubility**, Permeation
- Example: Situation for H in tungsten
- Discrepancy by factor of 60 between data from 1969 and 2001



I. Hydrogen transport in materials

Tritium retention and transport in material crucial

- Key parameters: Diffusion, Solubility, Permeation
- Limited database for fusion relevant materials (W, Be)
- No reliable uncertainty quantification even for fundamental properties
- Why?

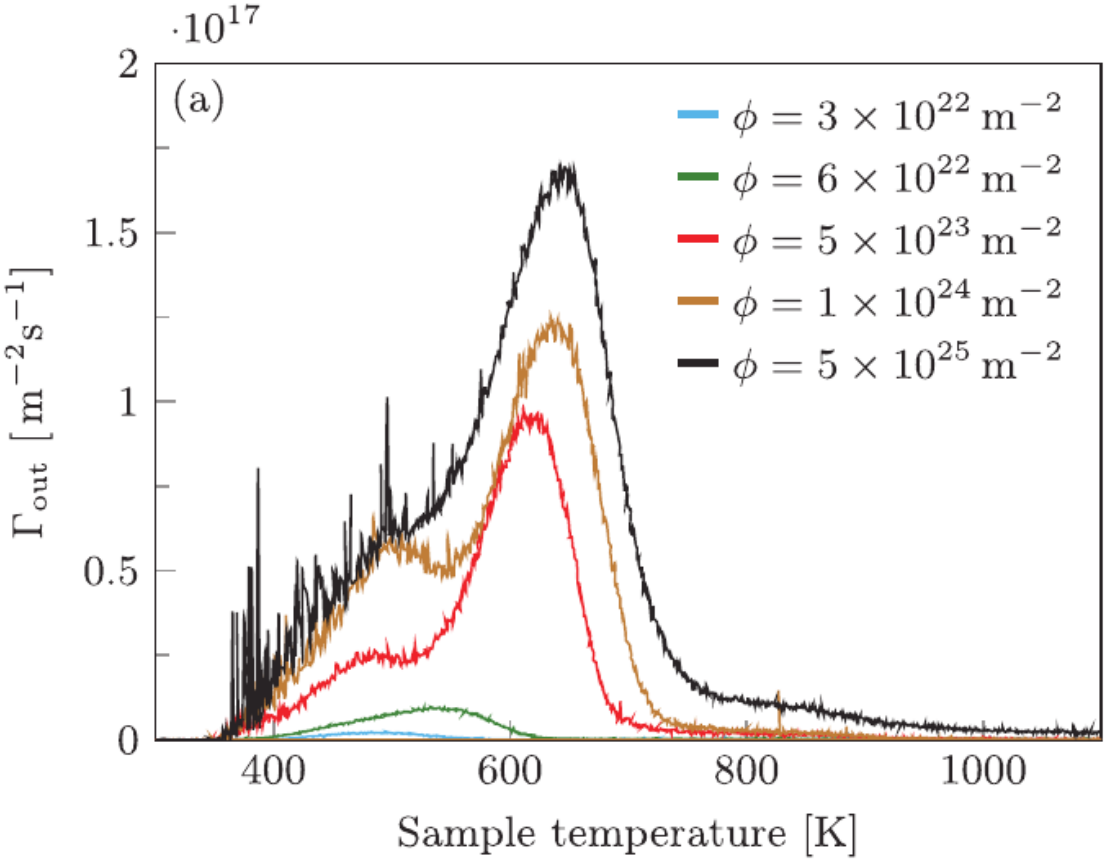
  Many reasons, eg. research focus in 70s different (hydrogen storage)

- Dedicated experiments with extended temperature range needed
  - In principle straightforward, but
    - High sensitivity needed
    - Measurements influenced by defects (trapping)
    - ...
- In addition:
  - Responsibility?

II. Hydrogen retention in materials

Tritium retention and transport

- Key parameters: trapping energies, trap density, trap distribution
- Experiment: Thermal desorption spectroscopy

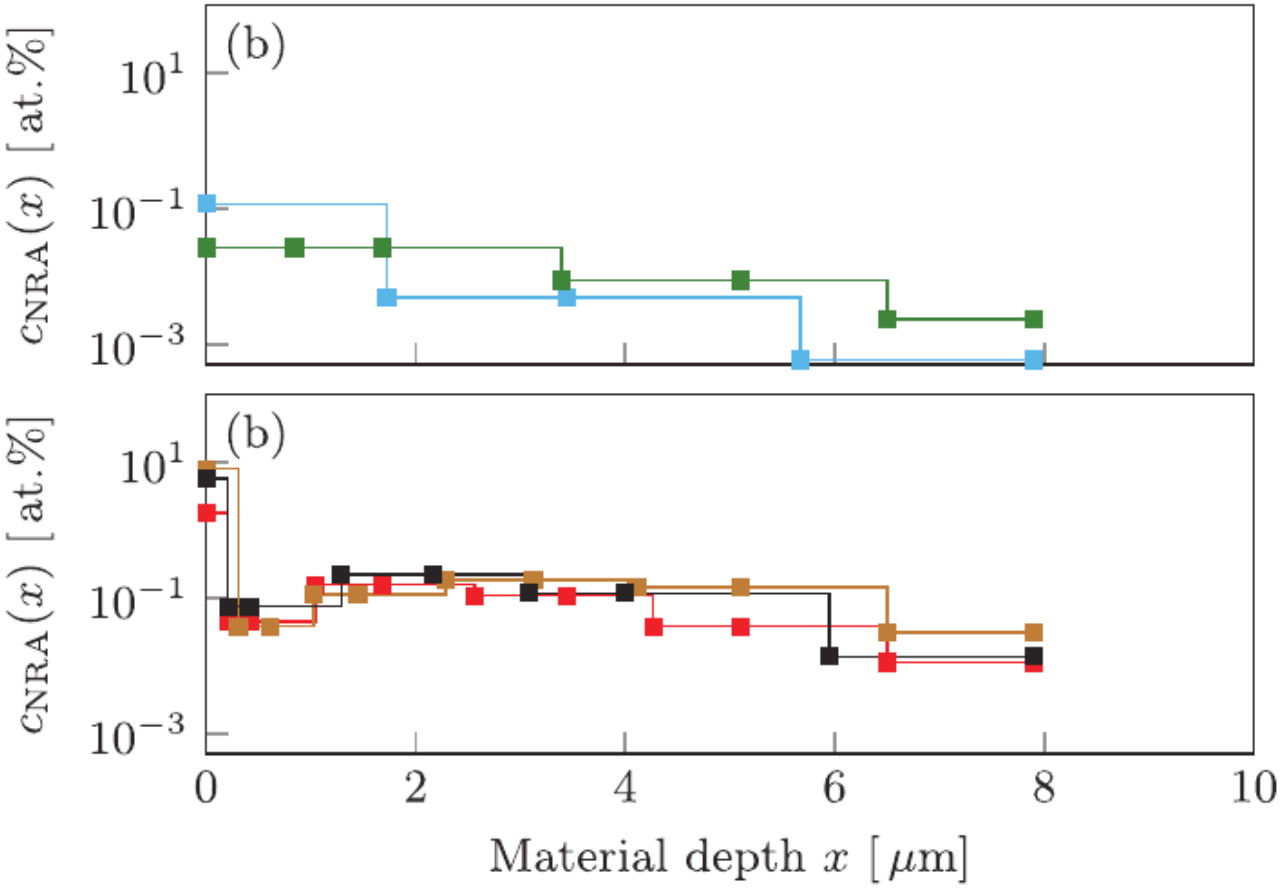


- Results are inconclusive: typically broad peaks – in literature 15 (!) different val.

II. Hydrogen retention in materials

Tritium retention and transport

- Effect of depth profile commonly neglected :-(

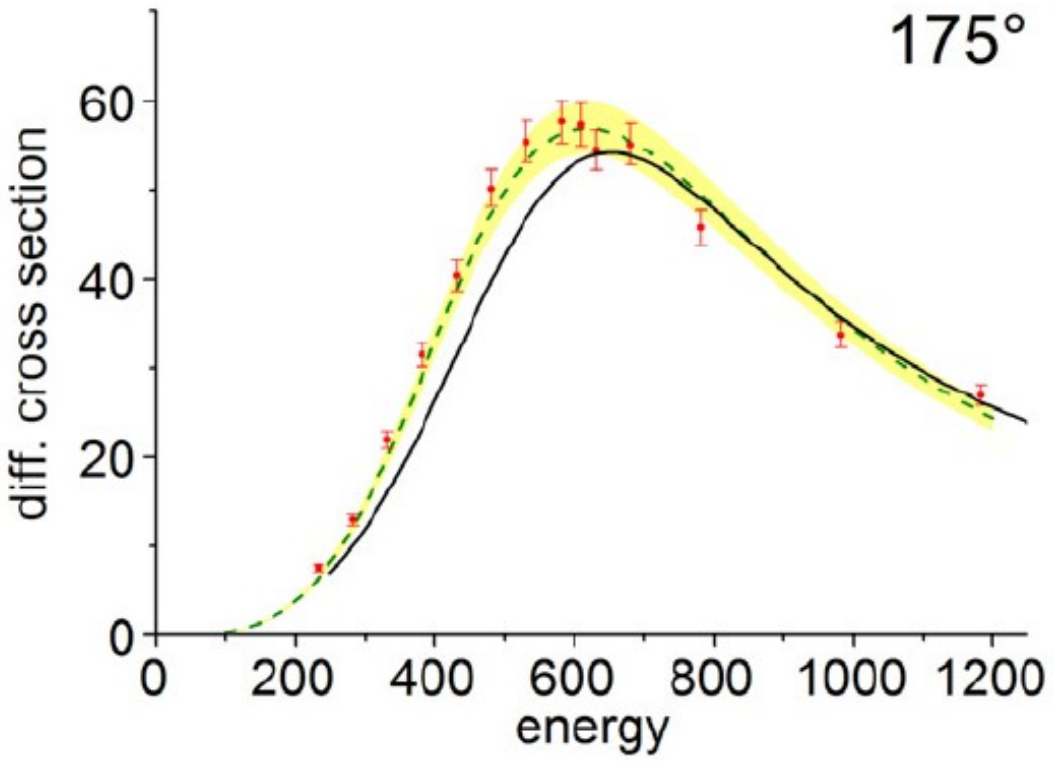


II. Hydrogen retention in materials

Tritium retention and transport

- Depth profile itself based on ill-conditioned inversion problem
  but old cross-sections were systematically shifted :-(

  (NIM B **371** (2016) 41)



II. Hydrogen retention in materials

Tritium retention and transport

- Trap energies are key component for retention and permeation modelling
- Present status not satisfying
- TDS evaluation challenging (ill-conditioned deconvolution problem)
- Atomistic parameters (ie. frequency-factor) typically set to fixed value (??)

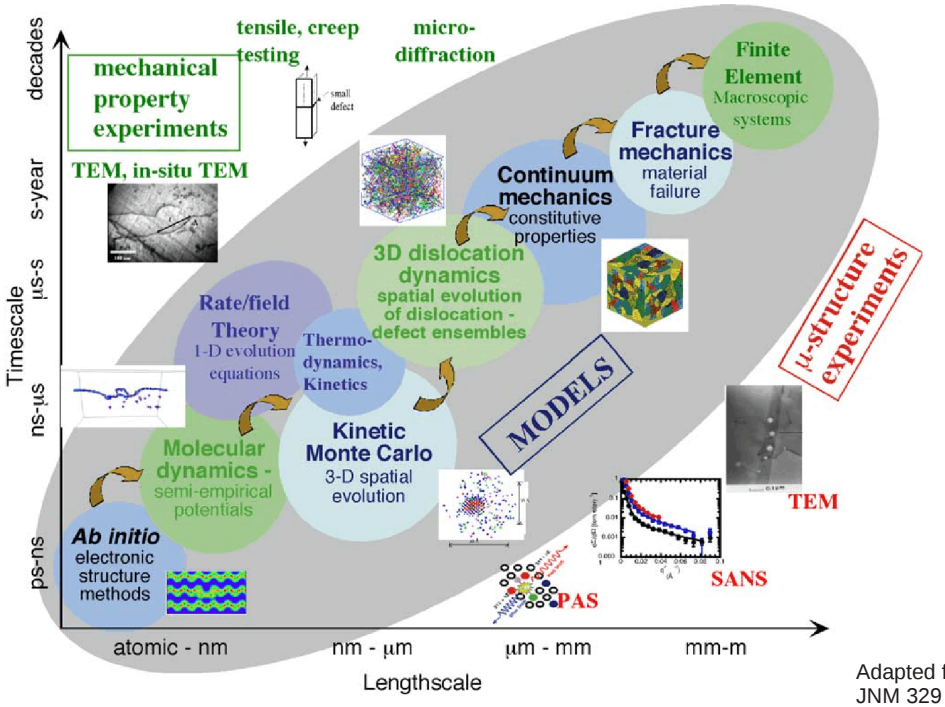
⇨ Round-robin experiments indicated

- Stronger modelling support needed (T>0 K)

III. Molecular Dynamic Potentials

Molecular dynamic simulations

- Simulation results depend on potential
- Standard approach: Fitting of parametric function to ab-initio/DFT/exp. data
- Parameter space high-dimensional: quality check – challenging
- MD-potentials at core of multiscale approaches



Adapted from B. Wirth, JNM 329 (2010), p. 103

Automated closed-loop potential development necessary

Approach based on Bayesian Gaussian processes appears feasible

Conclusion

Plasma.Material-Interaction:

- many basic data even for key materials are lacking or uncertain
- steel (i.e. EUROFER) as 'new' PWI material: next level of complexity of PMI – huge parameter space
- benchmarking and validation will be crucial (expect the unexpected)

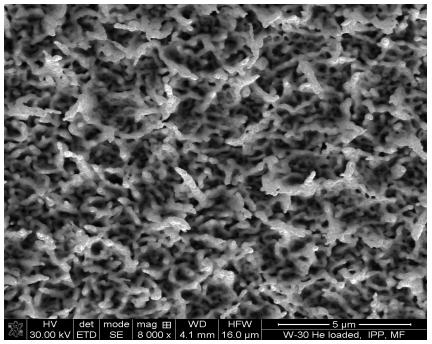
⇨ Strong need for joint experimental & modelling campaigns

⇨ Who is/ wants to be/ needs to be in charge?

Next level of complexity:

strong surface morphology development

GLADIS test: H. Greuner, H. Maier, M. Balden



5 µm

IV. Status and Outlook

Thank you
for your
attention

I. The atomistic level

Basis of all subsequent PMI effects: atomic collisions

- Collision events/cascades by impinging particles:

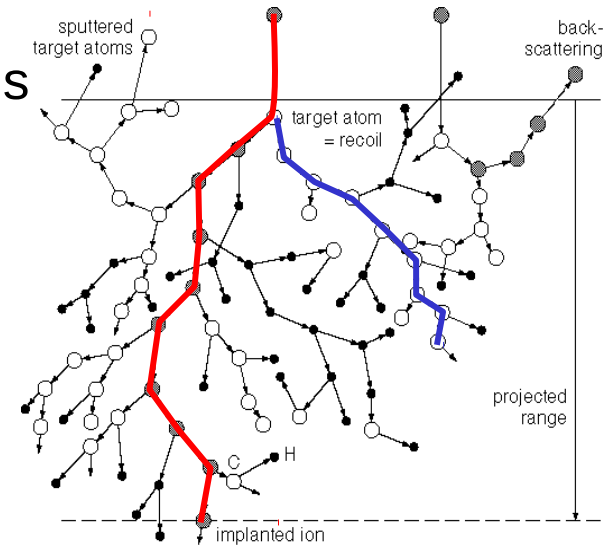
  - Displacements
  - Defect formation
  - Erosion due to physical sputtering

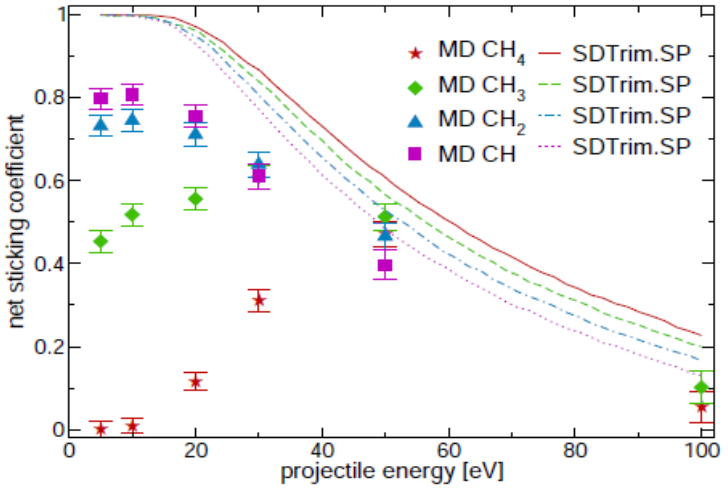
- Modelling tools:

  - Binary collision (BC) models (e.g. TRI
  - Molecular dynamic simulations

  MD alleviates restrictions of BC codes:

  - Low energy (< ~50 eV)
  - Molecules



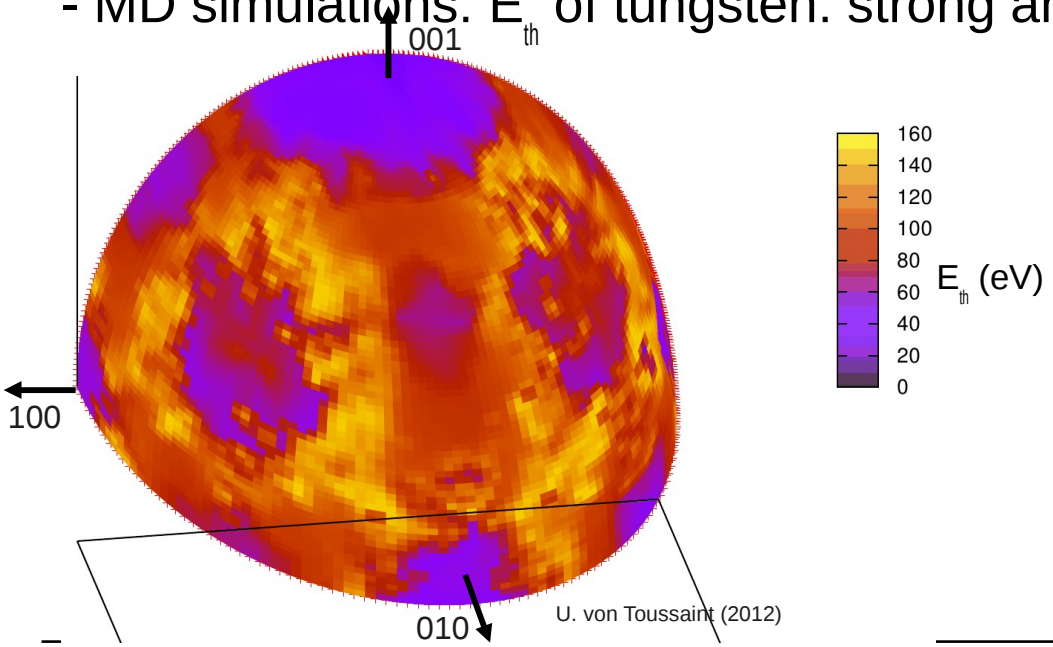


K. Tichmann, U. von Toussaint, W. Jacob, JNM 420 (2012), p. 291

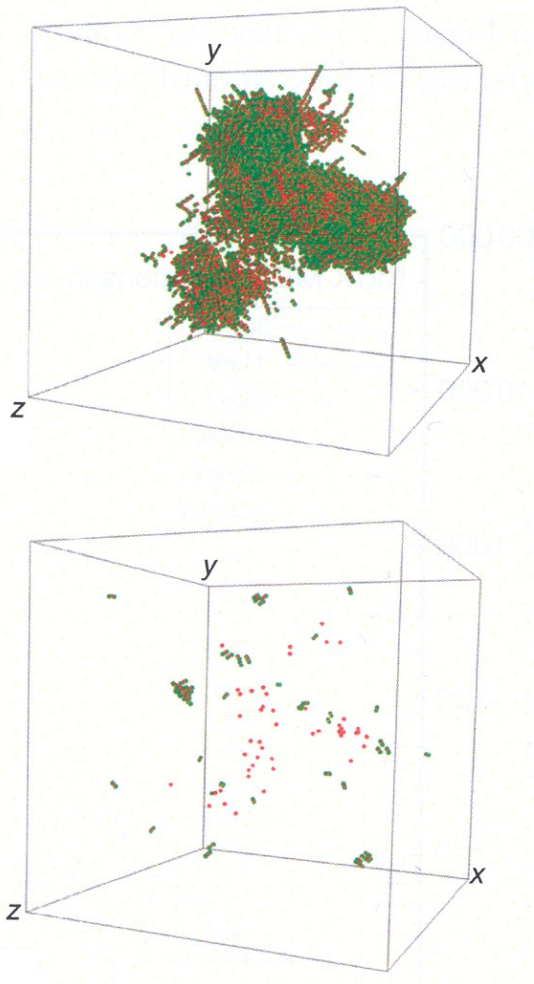
I. The atomistic level

Damage by energetic particles

- Number of displaced atoms:
  - NRT-model: $N_D = 0.8\, T_d(E) / (2E_{Th}) \sim E$
    - E_{th} =? (for tungsten: 40 eV, 90 eV,...)
    - Linear dependence correct?
- MD simulations: E_{th} of tungsten: strong anisotropy



U. von Toussaint (2012)



R.E. Stoller (2012)