Model TDS data using predictions from OKMC modeling

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J. Denis, Y. Ferro — PIIM, Aix-Marseille University, France

F. Granberg, J. Wu, T. Ahlgren — Department of Physics, Univerty of Helsinki, Finland

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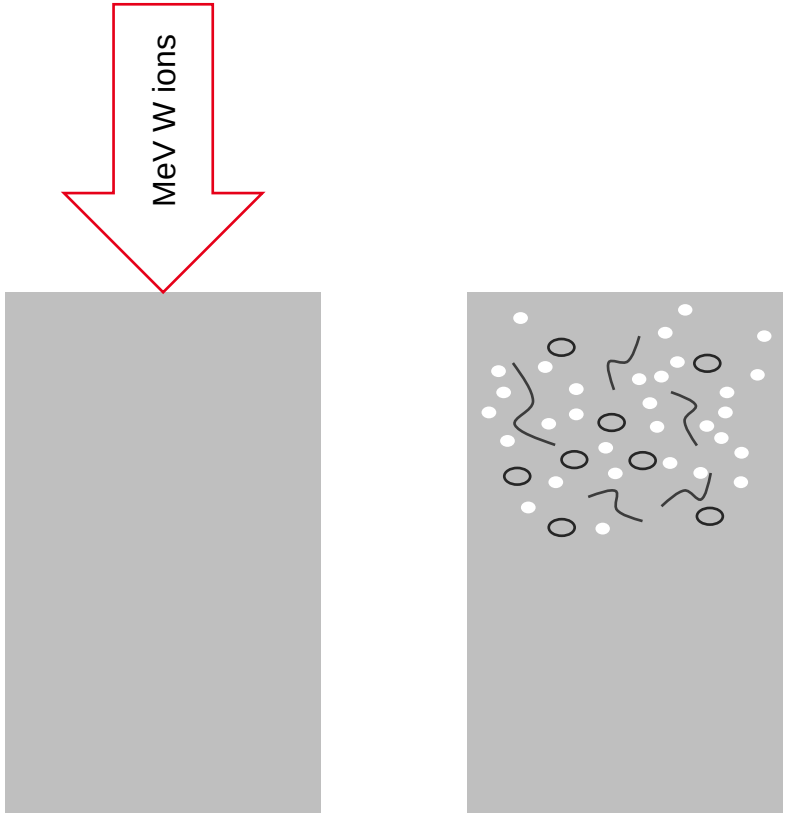
Context: D in self-damaged W

Self-damaged W mimics displacement damage created by neutron damage T. Schwarz-Selinger et al, Mater. Res. Express 10 (2023



Damaged zone (depends on the W ions energy, ~ µm)
vacancy clusters
Dislocations loops
Dislocations lines

Then this self-damaged zone is filled with D

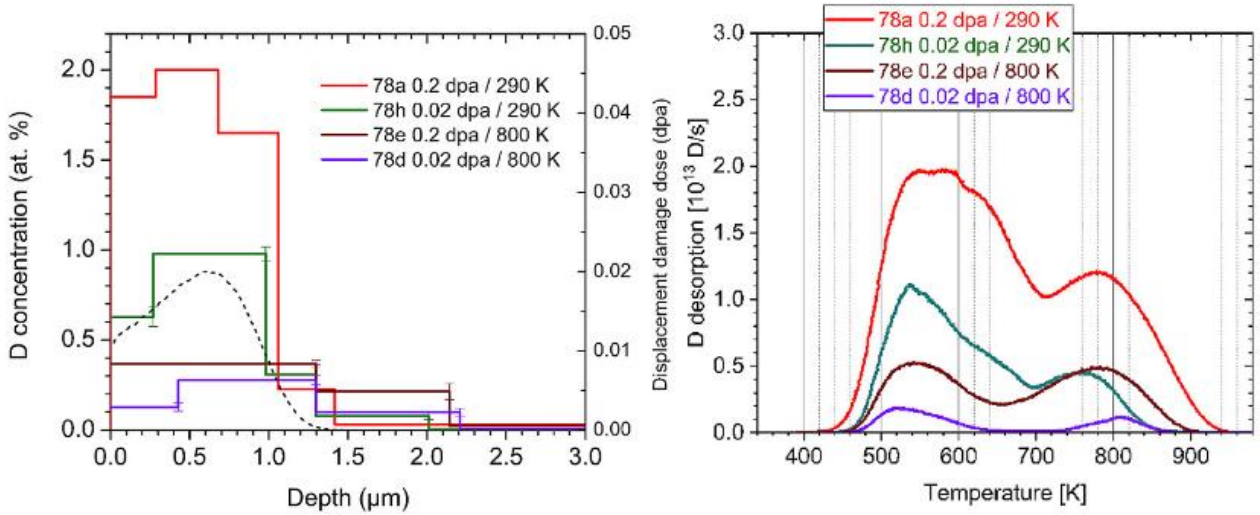
Context: D in self-damaged W

In experiments, basics of D in self-damaged:

high D retention in the damaged zone (~1.3 µm for 10.8 MeV, ~2.3 µm for 20.3 MeV)

2 peaks in TDS including high Temperature

Irradiation Temperature impacts defect concentrations: reduction 300 K -> 800 K



Single Crystal Tungsten

J. Zavasnik et al, Mater. Charac. 224 (2025)

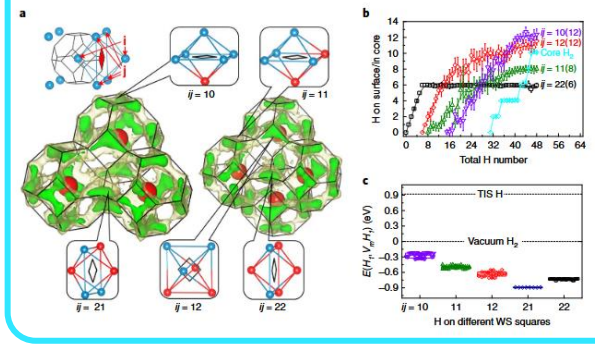
Context: D in self-damaged W

In Modelling: multi-scale

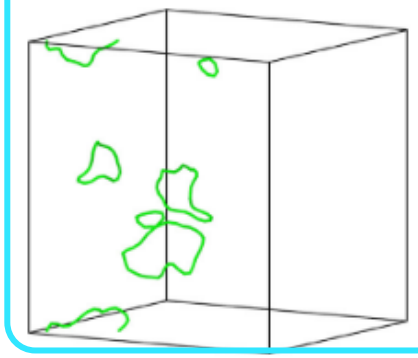
time

Distance

Density Functional Theory (DFT)
H in V_n
Hou et al, Nature Mater (2019)



Molecular dynamics (MD)
Dislocations in collision cascades
Granberg et al, JNM 556 (2021)



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Temperature evolution of radiation damage
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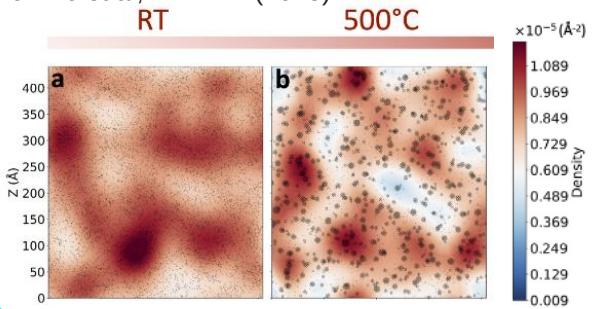
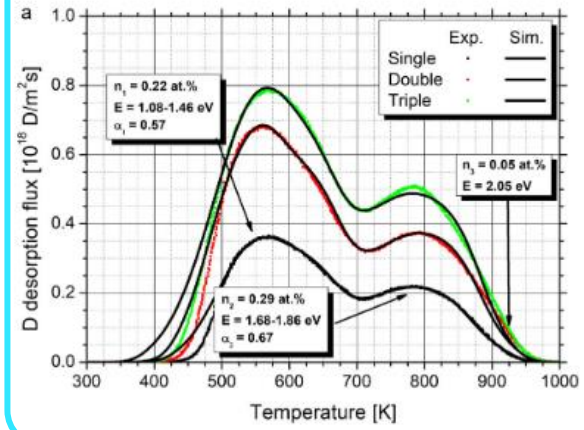


Rate equation modelling
TDS simulations with fitting E_{dt}
M. Pecovnik et al, JNM 550 (2021)



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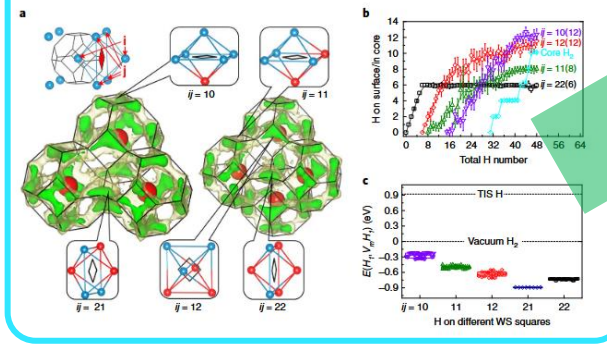

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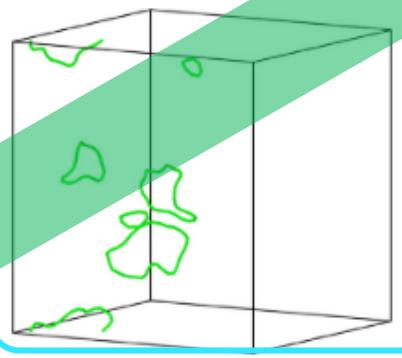

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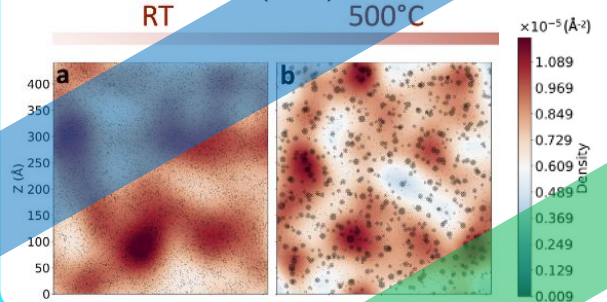

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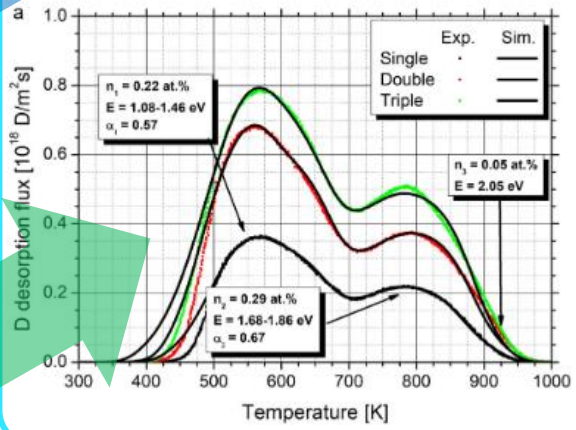

The "engineer" way: **a lot of work already published**
1. Reproduce the experiments with fitting parameters
2. Understand trends and defects with atomistic

The "physicist" way
1. DFT/MD/OKMC parametrize macroscopic models
2. Try to reproduce the experiments

Distance

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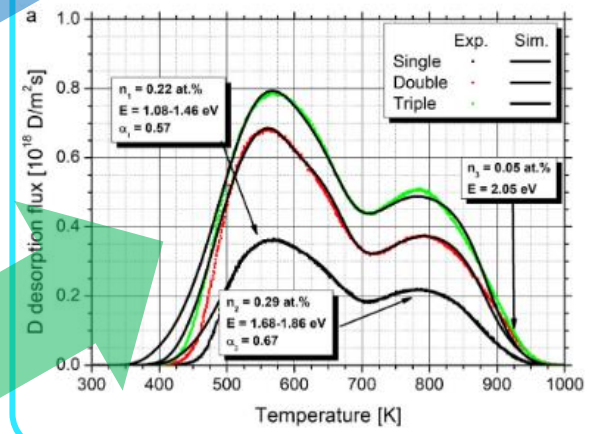

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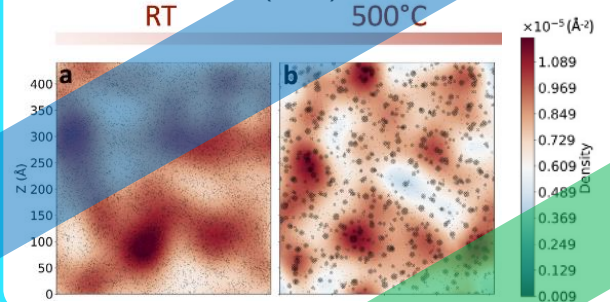

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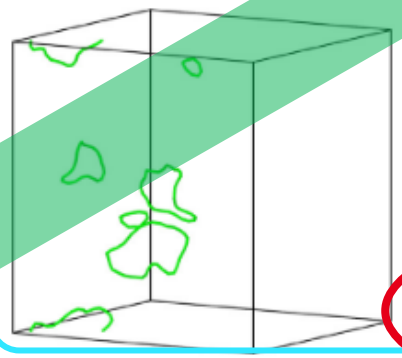

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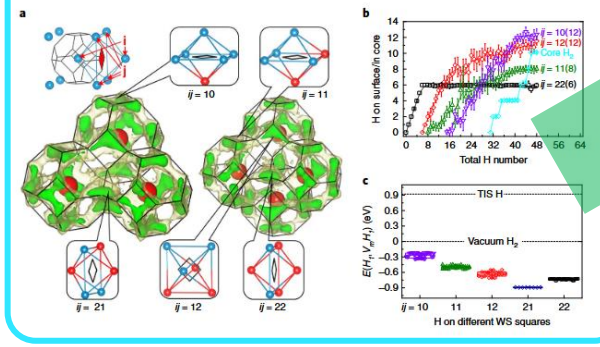

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today

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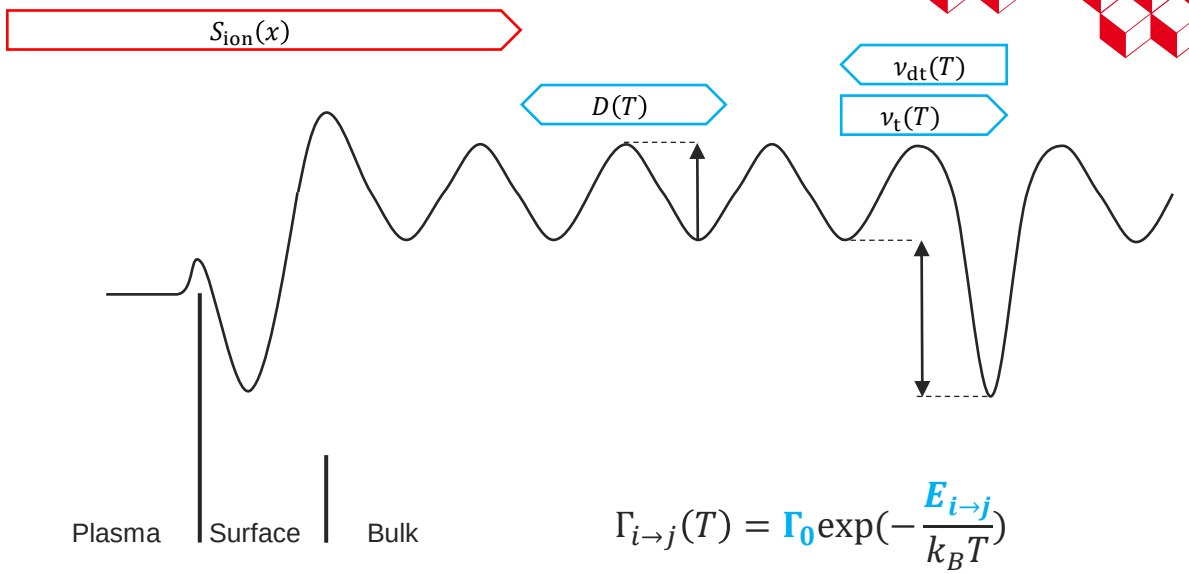
outline

1. **Macroscopic rate equation model**
2. **DFT based model and OKMC inputs**
3. **Toward cluster dynamics ?**

1. Macroscopic rate equation model

Governing equations



In the bulk :Two types of H:

- mobile (interstitial) c_{m}
- trapped (at defects) $c_{\mathrm{t},i}$

$$\frac{\partial c_{\mathrm{m}}}{\partial t} = \nabla \cdot (\boldsymbol{D(T)} \nabla c_{\mathrm{m}}) - \sum \frac{\partial c_{\mathrm{t},i}}{\partial t} + \boldsymbol{S_{\mathrm{ion}}(x)}$$

The total trap concentration of defect $\boldsymbol{i}$: $\boldsymbol{n_i} = \sum_{i=0}^{k} N_{\boldsymbol{i,j}}$

Defect $\boldsymbol{i}$ can trap $\boldsymbol{j}$ H (up to $k \geq 1$): $c_{\mathrm{t},\boldsymbol{i,j}} = \boldsymbol{j} N_{\boldsymbol{i,j}}$ with $N_{\boldsymbol{i,j}}$ the concentration of defect $\boldsymbol{i}$ with $\boldsymbol{j}$ H

For $j = 0$ $$\frac{\partial N_{i,j}}{dt} = -\boldsymbol{\nu_{\mathrm{t},j}(T)} c_{\mathrm{m}} N_{i,j} + \boldsymbol{\nu_{\mathrm{dt},j+1}(T)} N_{i,j+1}$$

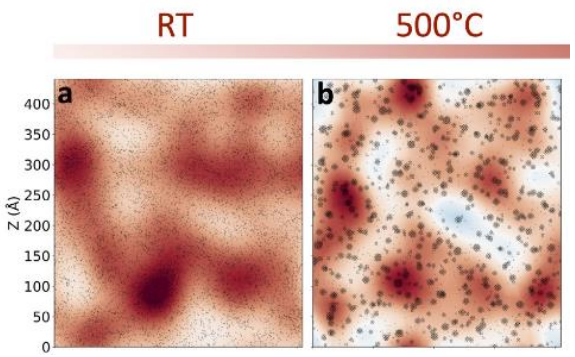
For $1 \leq j < k$ $$\frac{\partial N_{i,j}}{\partial t} = -\boldsymbol{\nu_{\mathrm{t},j}(T)} c_{\mathrm{m}} N_{i,j} - \boldsymbol{\nu_{\mathrm{dt},j}(T)} N_{i,j} + \boldsymbol{\nu_{\mathrm{t},j-1}(T)} c_{\mathrm{m}} N_{i,j-1} + \boldsymbol{\nu_{\mathrm{dt},j+1}(T)} N_{i,j+1}$$

For $j = k$ $$\frac{\partial N_{i,j}}{\partial t} = -\boldsymbol{\nu_{\mathrm{dt},j}(T)} N_{i,j} + \boldsymbol{\nu_{\mathrm{t},j-1}(T)} c_{\mathrm{m}} N_{i,j-1}$$

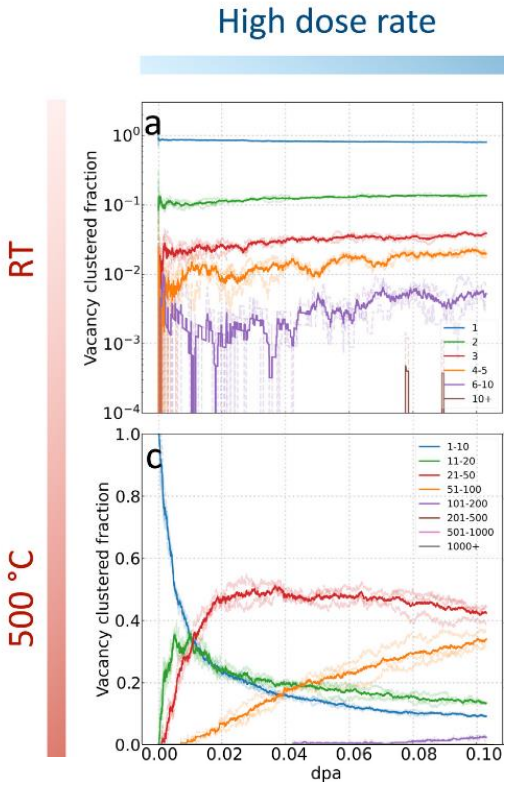
From atomistic model/calculations

2. DFT based model and OKMC inputs

Inputs of the model



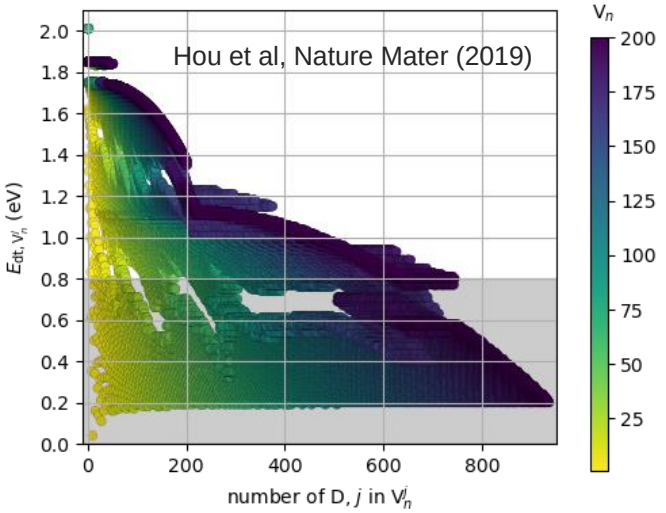
Object Kinetic Monte Carlo
Temperature evolution of radiation damage
J. Wu et al, NME 44 (2025)



MHIMS Input:
n_i trap concentration

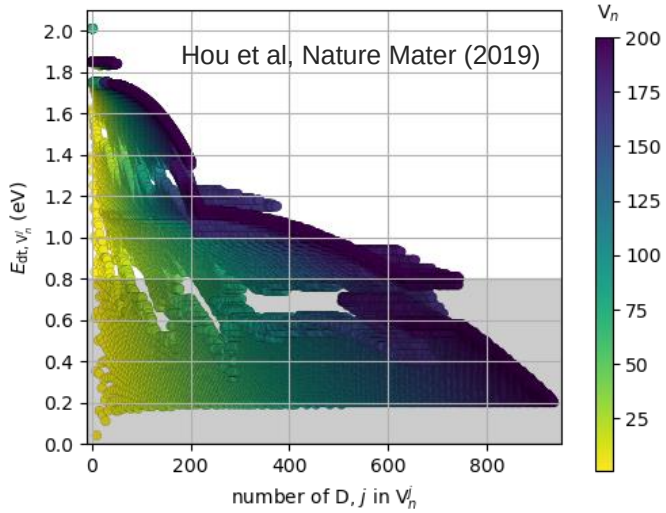
Damaging at 300 K:
Mainly V1, up to V10+

Damaging at 800K:
Up to V_{200}



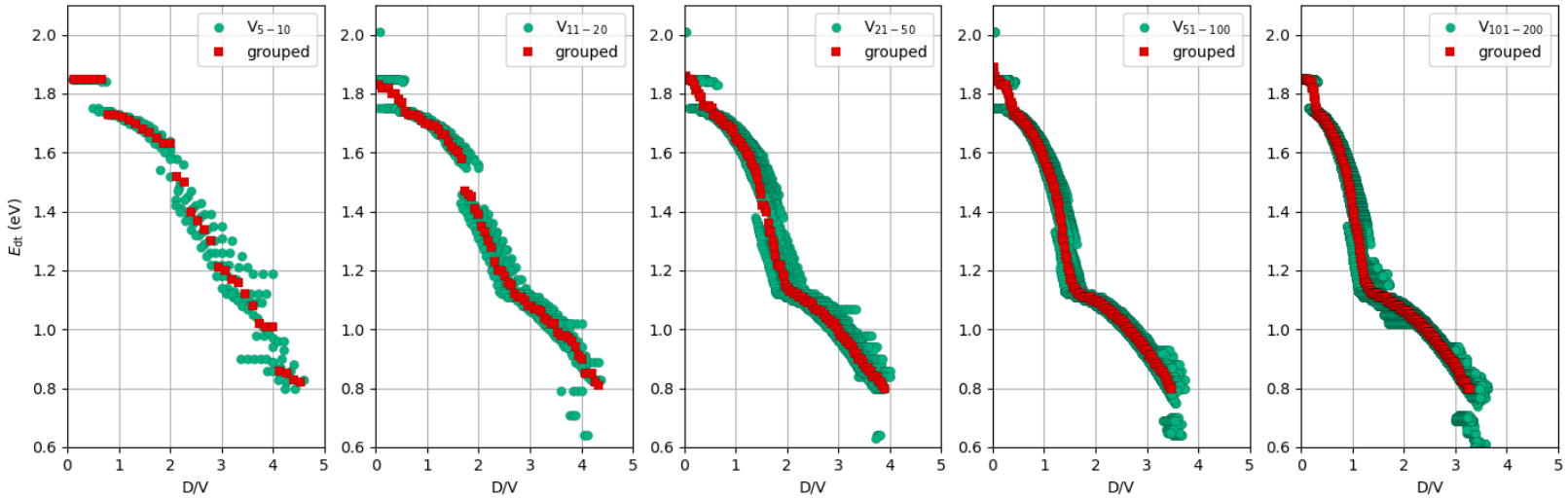
Too much E_{dt}
96,000 equations per mesh element
⇒ grouping V_n

Inputs of the model



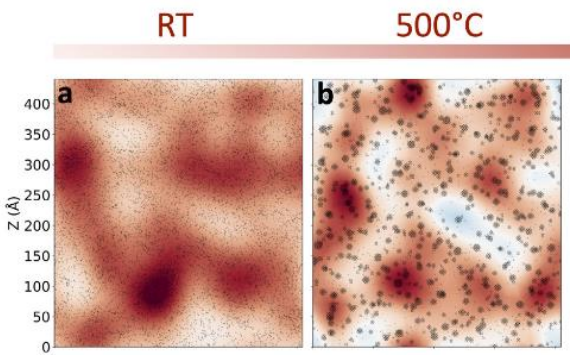
Too much E_{dt}
70,000 equations per mesh element
⇒ grouping V_n

⇒ grouping V_n
Managable E_{dt}
~1000 equations per mesh element



MHIMS Input:
$E_{i \to j}$ detrapping energy

Inputs of the model



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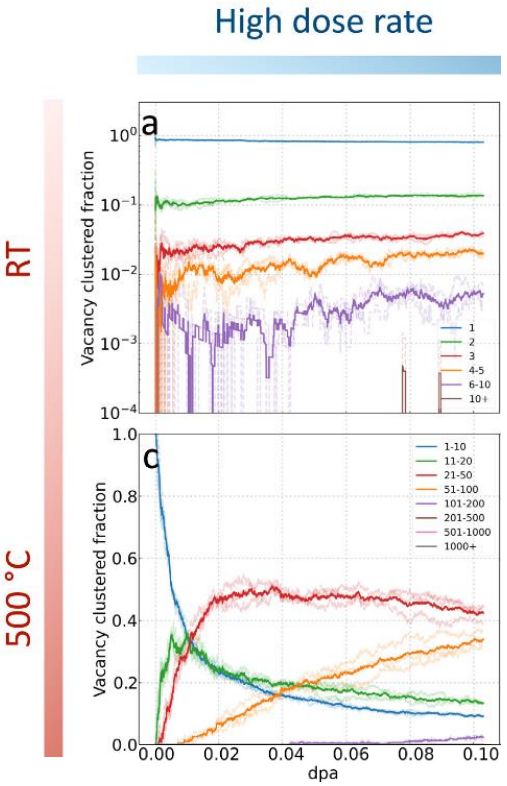
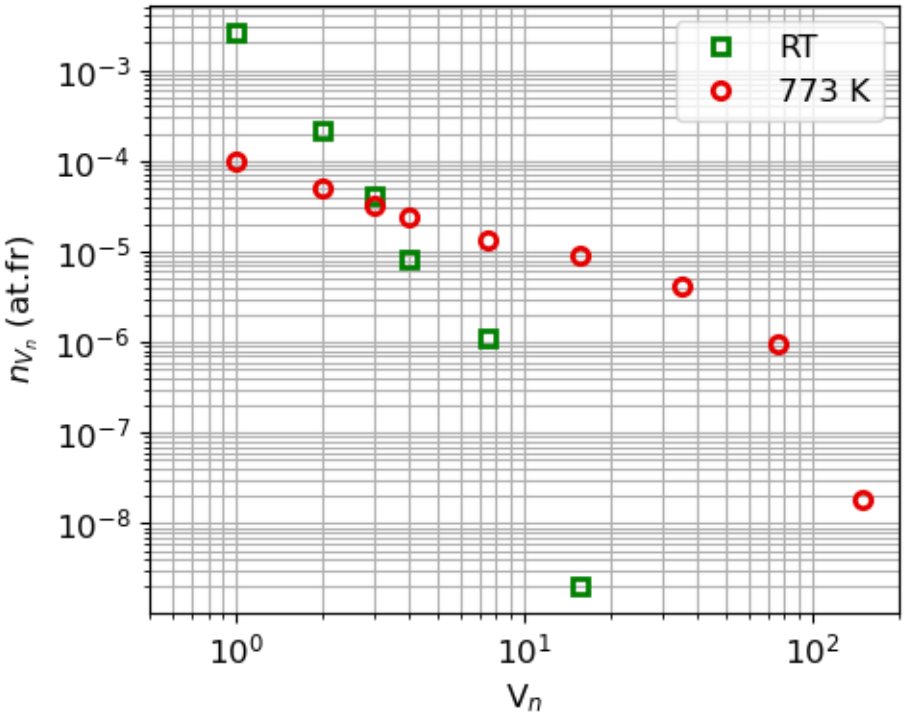




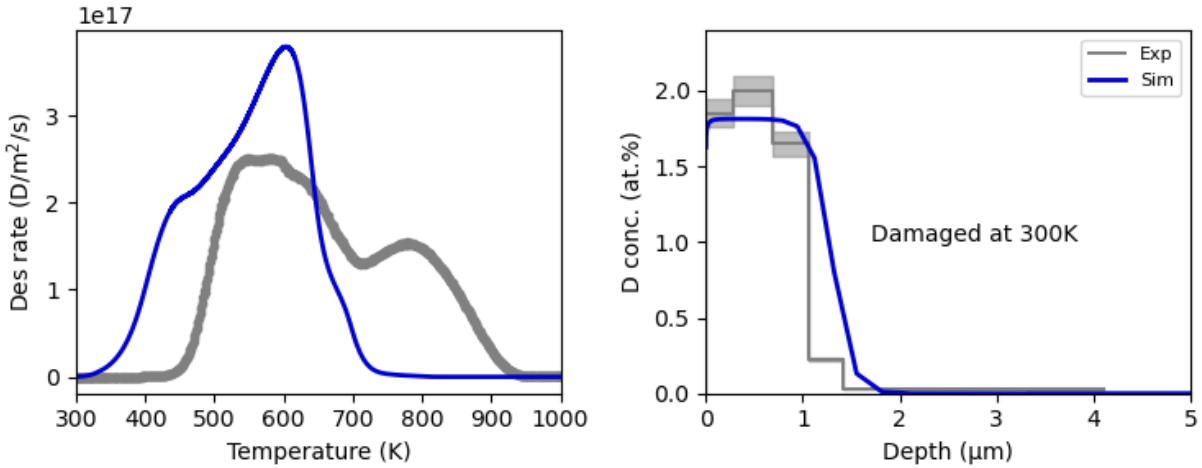
Relative distribution given by OKMC

Absolute quantity adjusted to reproduce NRA concentration

Comparison with experimental results

Experiment from J. Zavasnik et al, Mater. Charac. 224 (2025)

self-damaged W (300 K and 800 K) exposed to 5 eV/D, 6×10^{19} $Dm^{-2}s^{-1}$ for 48 h at 370 K



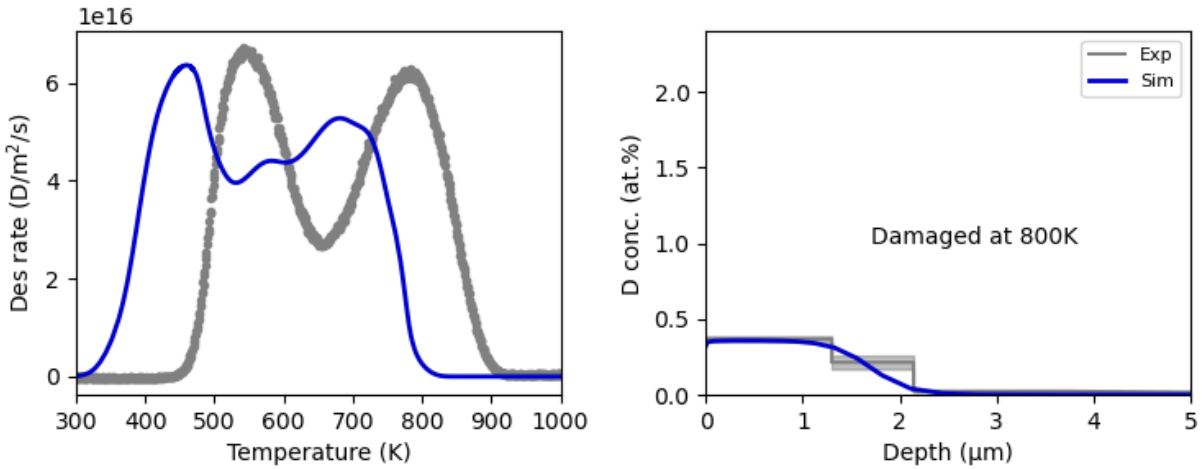
Damaged at 300 K

First Peak: OK but too high

No 2nd peak !

PAS-DB: presence V_2-V_4

OKMC predicts mainly V_1



Damaged at 800 K

Two peak features with same intensity

Shifted towards low Temp

DFT accuracy ?

experimental temperature

Comparison with experimental results

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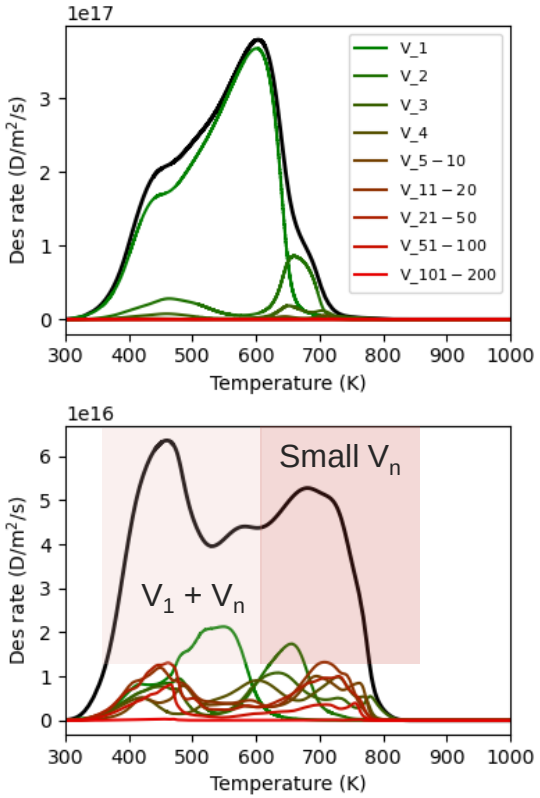
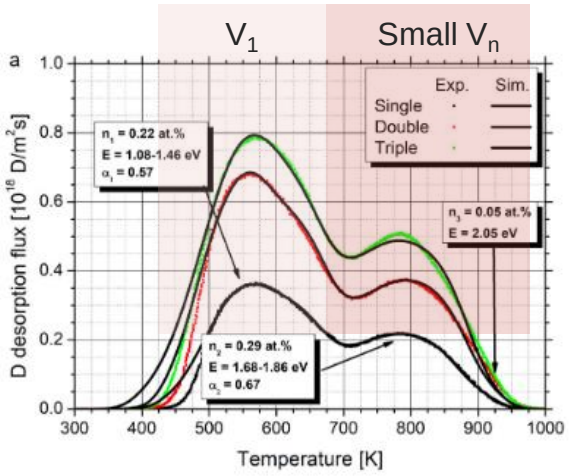
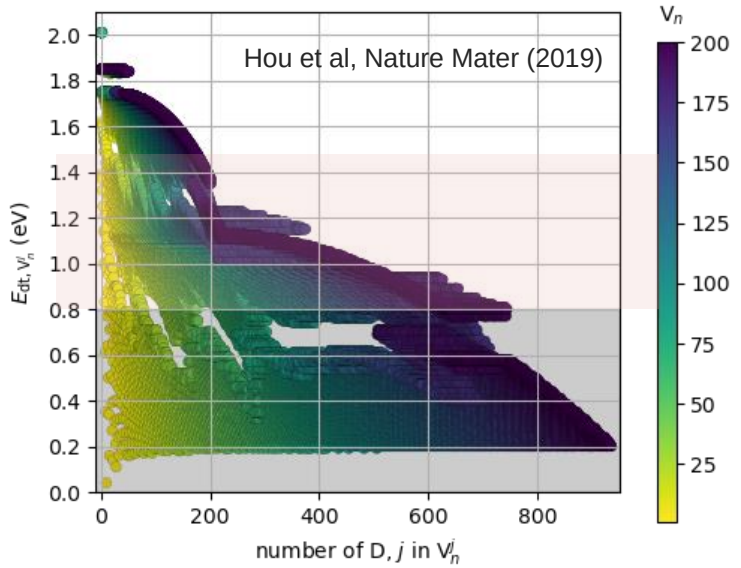
"physicist" way



"engineer" way



M. Pecovnik et al, JNM 550 (2021)

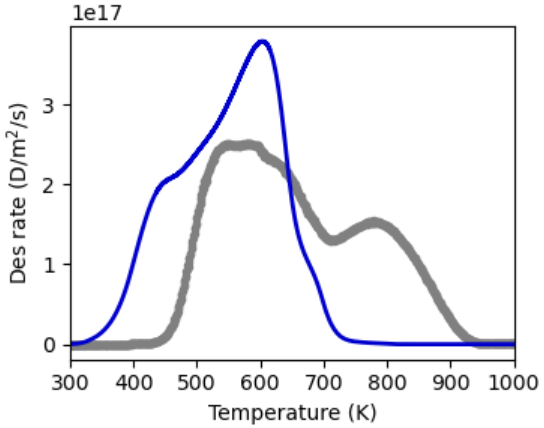


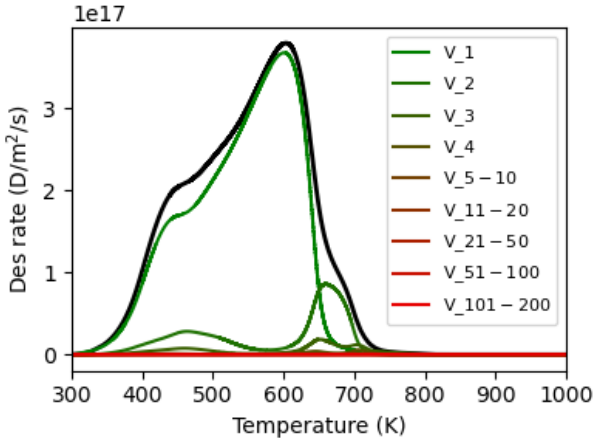
Different interpretation:
First peak not only V_1 BUT ALSO $V_{n>1}$

3. Toward cluster dynamics ?

Comparison with experimental results

Damaged at 300 K: Why only contribution of V_1 ?





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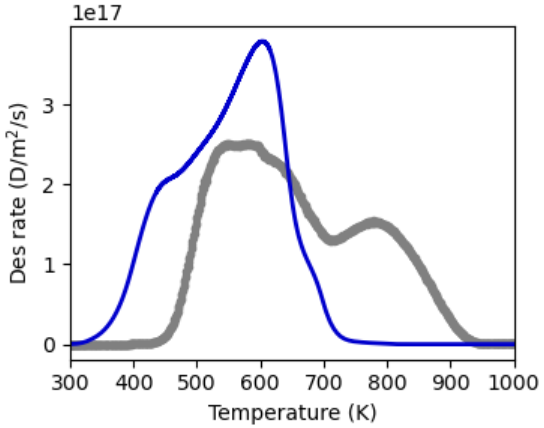
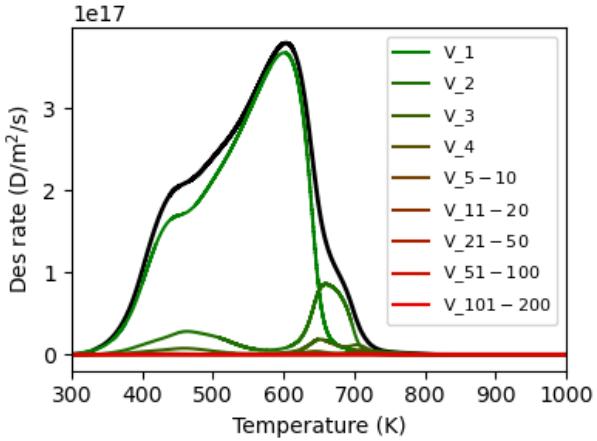
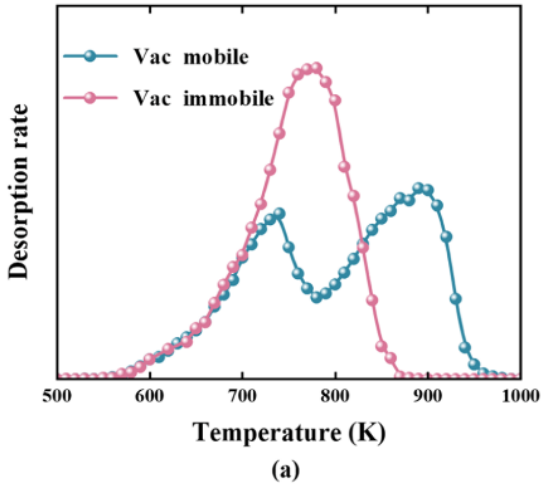
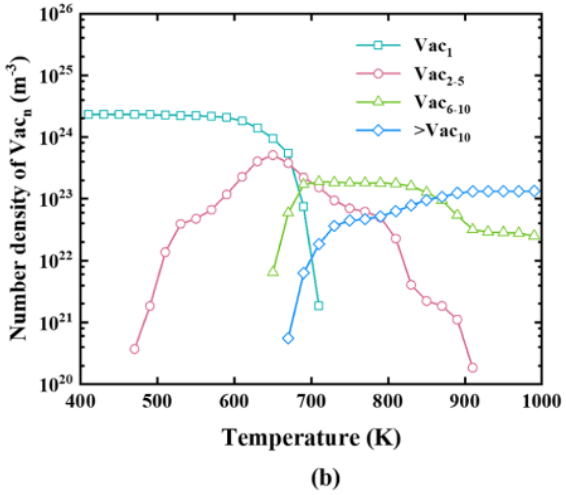




OKMC simulations allowing V_n clustering

Ma et al. Acta Mater. 294 (2025) 121130





What happen if V_n clustering is added to the Rate Equation models ?

Adding simple cluster dynamics aspects

ADDING to MHIMS:

Clustering: $V_n + V_j \rightarrow V_{n+j}$

Annealing with Insterstitial loop: $V_n + I_{\text{loop}} \rightarrow I_{\text{loop}}$ (but less Interstital)

Reaction rate based on Diffusion coef (But Diff of V_n not explicitely taken into account)

Simulating experiment from Pecovnik et al, JNM 550 (2021)

self-damaged W 300 K, exposed to 5 eV/D, 5.9×10^{19} $Dm^{-2}s^{-1}$ for 74 h at 370 K

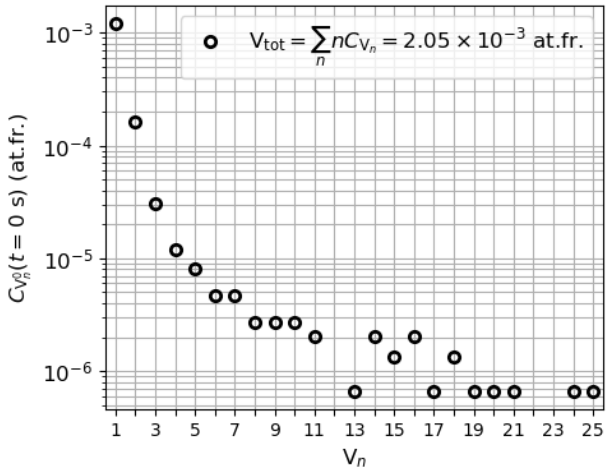
Inputs: No free parameters

Trap concentration: MD [Granberg et al, JNM 556 (2021)]

Detrapping energies: DFT-based model [Hou et al, Nature Mater (2019)]

Adding simple cluster dynamics aspects

Granberg et al, JNM 556 (2021)



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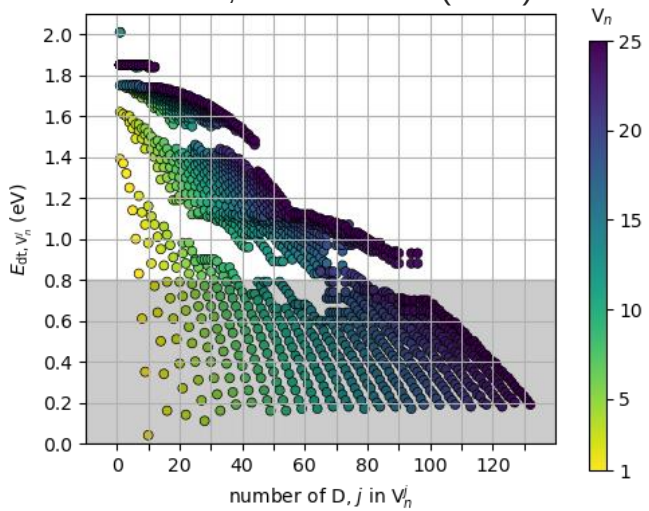
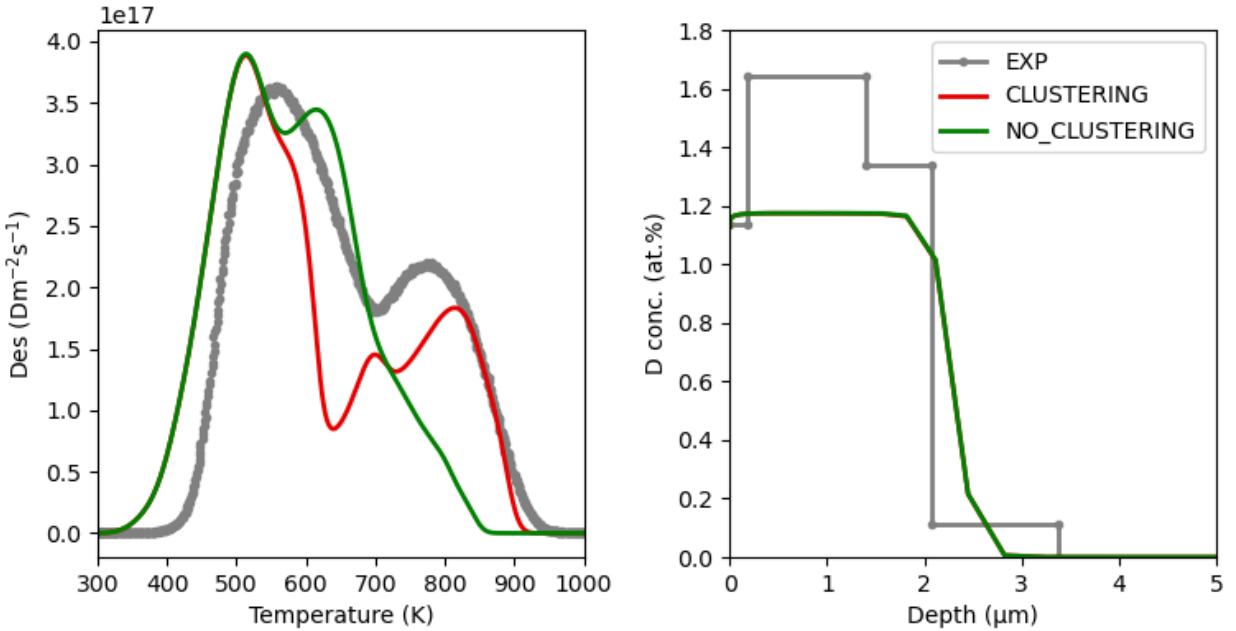




Around 600 K, V_1 transforms into bigger V_n and D is not fully desorbed
⇒ creates the 2nd peak in the TDS

TDS affects the nature of the damage layer (same as in EUROFer Schmid et al, NME 34 (2023))

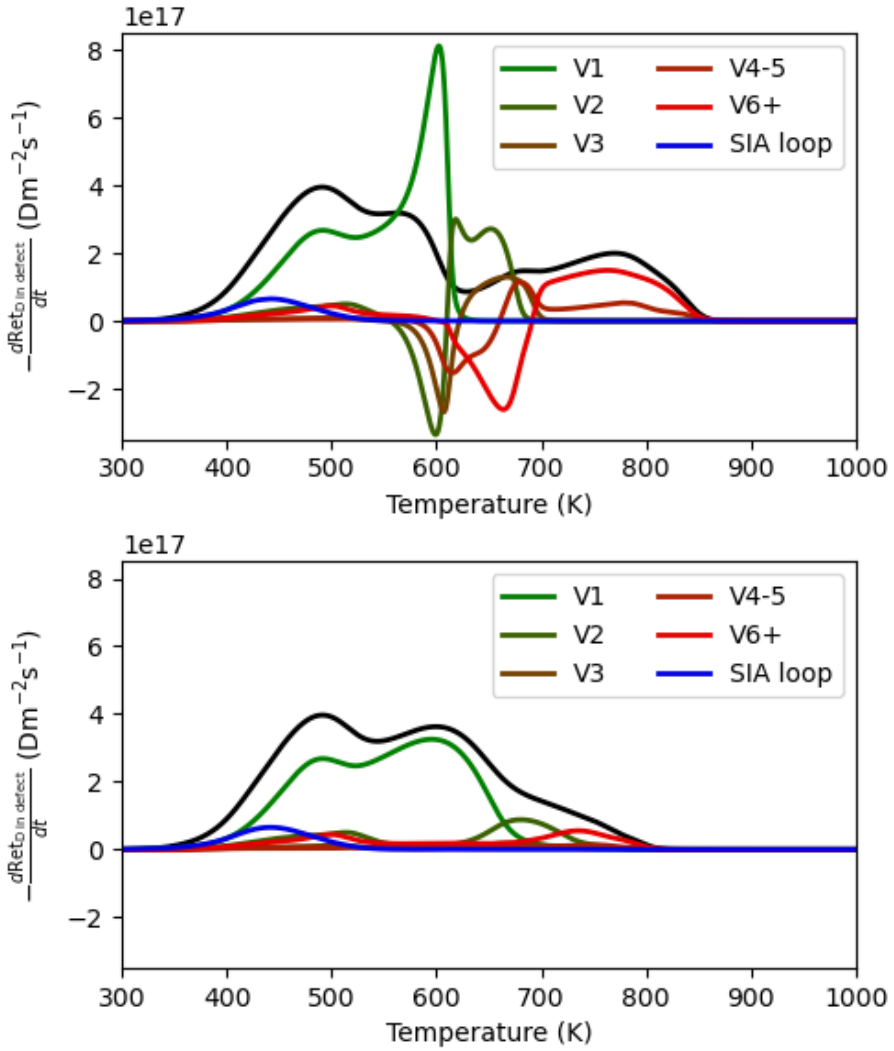
CONCLUSIONS

Conclusions

- OKMC + DFT based model with "physicist" way:
  - Allow to reproduce the main feature of experimental TDS
  - All Vn sizes contributed to the First peak, not only V1: extend the interpretation of the "engineer" way
  - BUT TDS after damaging at 300 K: no 2nd peak in the TDS
    - V_2-V_4 seen in PAS but mainly V_1 in OKMC

- Adding clustering of Vn allow to have a 2nd peak in the TDS:
  - Around 500K-600K V1 transform into Vn>1 creating deeper trapping site for the D still in the sample
  - TDS affects self-damaged W (similar to damaged EUROFer)

Adding simple cluster dynamics aspects



Around 600 K,

$V_1^0 + V_1^j \rightarrow V_2^j$ (and after $V_{n>1}$)

⇒ creates deeper trapping site and D stay a bit longer in the sample

600 K and not earlier because only empty V_1 can "move" to cluster