# Verification of codes with permeation simulations

Material: Tungsten

Atomic density:  **Wm-3**

Tetrahedral interstitial site (TIS) density:

Diffusion **m2s-1**

Solubility **H/W Pa-1/2**

Trap parameters:

There are 3 trap types in the simulations:

Trap 1 and trap 2 are intrinsic traps:

Trap 3 is close to the surface: with nm and nm.

For each trap, the trapping energy is the diffusion energy eV.

For each trap, the pre-exponential frequency for trapping ( indices) and detrapping ( indices)are  **s-1**

The detrapping energy and trap concentration are obtained through a parametric optimization. Thus, there are 6 parameters to determine.

Boundary conditions:

At both sides of the material, a Dirichlet Boundary recombination is used. It represents the case where the recombination is not limiting the desorption of D.

Sample and exposure conditions:

We want to simulate the experimental results described in [Ogorodnikova, Roth and Mayer, Deuterium retention in tungsten in dependence of the surface conditions, J. Nucl. Mater. 313-316 (2003) 469-477]. The TDS spectra to be simulated is given in figure 5 of this reference (fluence 1023 D/m2).

Thickness:  **µm**

Exposure condition and TDS:

1. 200 eV/D implantation, D/m2/s at 300 K for 4000 seconds: if the reflection coefficient of the ions is considered to be around 0.5 for normal incidence, the incident fluence is 1023 D/m2.
2. A storage phase at 300 K (no flux, atoms or molecules)
3. A TDS steps with a ramp of 8 K/s: from 300 K to 1100 K in 100 secondsack side)

Results:

The optimization on the 6 parameters leads to the set of following parameters for a relative error of 2.91%:

|  |  |  |  |
| --- | --- | --- | --- |
|  | Trap 1 | Trap 2 | Trap 3 |
| (eV) | 0.834 | 0.959 | 1.496 |
| (at.fr.) | 1.364×10-3 | 3.629×10-4 | 9.743 ×10-2 |

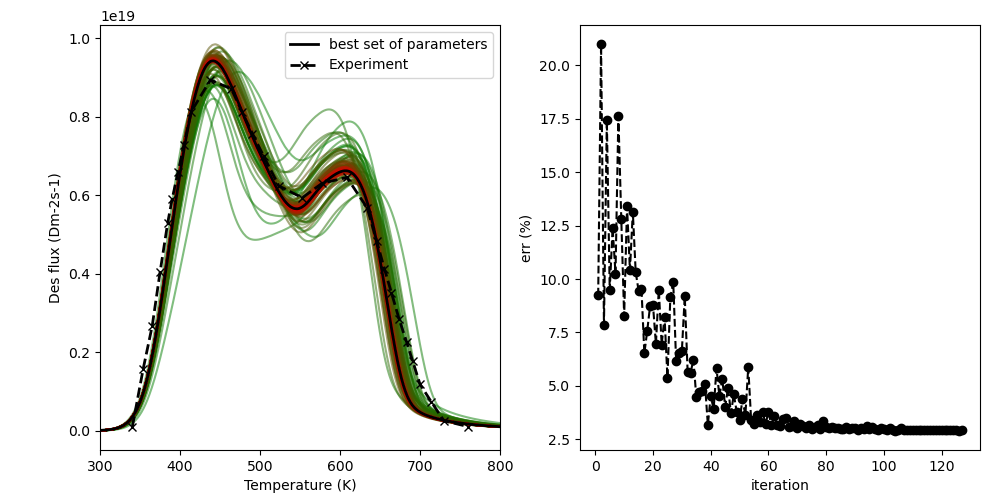


Figure 1. left) comparison between the simulation and the experiments during the optimization process. Right) evolution of the error () during the optimization.

This results are not far from the calculated value I obtained in the first MHIMS paper [Hodille et al., J. Nucl. Mater. 467 (2015) 424-431] (I was then using the experimental results of the lower fluence shown in the paper by Ogordnikova, Roth and Mayer). In my PhD thesis, I also simulated this data and come up with similar trapping parameters (0.85 eV/1.3×10-3 at.fr., 1.00 eV/4×10-4 at.fr. and 1.5 eV for the surface trap) that I used as initial guesses for the optimization. At that time, I was not doing the optimization automatically so my results could have been not optimized.