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MHIMS multi-isotopes modelling applied to Eurofer97 TDS

Predicting accurately the permeation and retention of tritium in plasma-facing components is key to ensure the safety and the viability of future fusion reactors. This prediction relies on numerical modelling that itself requires experimental validation.
To obtain such a model for diffusion and trapping in Eurofer97, a coupled modelling of hydrogen permeation and deuterium TDS experiments was performed. This analysis conducted using the reaction-diffusion code MHIMS [1] yielded a model including three trapping sites, with detrapping energies 0.51 eV, 1.27 eV and 1.65 eV [2]. These simulations were performed with a single-isotope version of MHIMS. However, the experimental TDS spectra show that D2 is not the only species that desorbs from the sample: a non-negligible signal corresponding to the desorption of HD is recorded, coming from the native amount of hydrogen contained in Eurofer97. Furthermore, the proportion of HD vs. D2 that desorbs varies depending on the trapping site: schematically, D2 desorbs from the lower-energy trapping site while HD populates the higher-energy trapping site.
To cover this, new TDS experiments are presented along with the corresponding simulations, obtained with the multi-isotope version of MHIMS. In particular, an initial H2 loading step is added to the simulation scenario to account for the native H2 content found in Eurofer97 samples, as measured with catharometry. However, in simulations performed with the three-trapping sites model, this hydrogen content is totally depleted during the deuterium loading phase (4 hours at 450℃ under D2 atmosphere) and replaced with deuterium. Consequently, there is no HD desorption in the subsequent TDS simulation, which is in contradiction with the experimental observations that motivate the analysis. Therefore, a trapping site with a higher energy is required for the model to correctly simulate the HD desorption that is witnessed at higher temperatures.
The presentation will cover a new set of TDS experiments that were performed to study the D2 vs HD desorption depending on the loading conditions (temperature, duration), as well as the changes proposed to the three-trapping sites MHIMS model for diffusion and trapping in Eurofer97 in order to get a satisfying simulation of the multi-isotope behaviour.

[1] Hodille, E. A., et al. “Deuterium uptake, desorption and sputtering from W (110) surface covered with oxygen.” Nuclear Fusion 64.4 (2024): 046022.
[2] Montupet-Leblond, Floriane, et al. “Influence of traps reversibility on hydrogen permeation and retention in Eurofer97.” Nuclear Fusion 62.8 (2022): 086011.

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