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Bridging model and real systems with laboratory experiments: dynamic retention of deuterium in tungsten

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In this contribution we will present our laboratory experimental approach, which has been especially developed to ease the comparison with DFT calculations and other modeling methods. Not only we want to quantify accurately e.g. deuterium dynamic retention but we also strive to understand the chemical and physical origin of deuterium and tungsten interactions. To this end, we have built an apparatus allowing preparation of tungsten samples, ionic implantation of deuterium with various fluxes and quantification of deuterium retention, everything being performed *in-situ* in ultrahigh vacuum. For precise quantification of deuterium retention, a state-of-the-art differentially pumped Temperature Programmed Desorption (TPD aka TDS) system has been designed allowing sub-monolayer sensitivity i.e. once the implantation depth is taken into account we are able to study fuel retention down to very low deuterium atomic densities (10^{-5} and below). This sensitivity eases the comparison with theoretical methods and will help to decipher surface effects in retention/release processes in model materials such as low defect density poly- and single crystals.

As an example of the power of this experimental approach, the study of the dynamic retention of deuterium in a model tungsten material will be presented. Dynamic retention is a process where release of retained fuel can be delayed from a tokamak plasma discharge, i.e. during reactor down-time, and can account for large portion of the fuel inventory [1].

With our new *all-in-situ* apparatus, we first measured deuterium retention for low fluences in the 10^{17} D/m^2 to 10^{21} D/m^2 range, extending the available literature explored range to nine orders of magnitude. Second, we demonstrate that the release of deuterium from tungsten occurs at room temperature and accounts for more than two thirds of the loss of implanted fuels on timescales typically of hours and days. Third, the evolution of TPD spectra as a function of waiting time in vacuum at 300 K strongly suggest that several binding energies are associated with deuterium retention in low defect density tungsten, *even when a single TPD desorption peak is measured with TPD*. These laboratory observations can be well explained by Density Functional Theory (DFT) calculation that models the trapping of several deuterium atoms on a single tungsten vacancy.

[1] Loarer *et al.*, Nucl. Fusion 47, (2007) 1112