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Comparison of a quantitative diffusion-trapping model with experiments on D uptake in damaged W

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Uptake of deuterium into defect rich tungsten was studied experimentally as a function of temperature and D fluence as a test case to compare quantitatively with modelling. First recrystallized W samples are implanted with 20 MeV W^{6+} ions. This creates a damaged layer of about 2.5 µm thickness. Subsequently, these samples are exposed to low-temperature deuterium plasmas to decorate the defects created by W^{6+} irradiation. In order to avoid further modification of the samples during plasma exposure due to impinging ions with sufficient energy to create displacements, the exposure is typically performed at floating potential. Under these conditions, the impinging ions are predominantly D_3^+ with a kinetic energy of 15 eV, respectively 5 eV/D. The ion flux is about $6x10^{19}$ D/m²s under these "gentle" loading conditions. The experimental procedure furthermore consists of depth profiling of the retained D by nuclear reaction analysis (NRA), as well as the quantification of the total D amount and the investigation of D binding energies by temperature programmed desorption (TPD).

These experiments are an ideal benchmarking case for a diffusion-trapping code TESSIM[1*]. They provide comparatively large and easily measurable deuterium inventories in a well-defined volume (i.e., the damaged layer). Furthermore, the samples do not change their trap density profiles during plasma exposure. For our benchmark, calculated D depth profiles after implantation as well as TPD spectra are quantitatively compared to experimental results. We try to minimise the number of free parameters in the model, with the goal being self-consistent and predictive. Our test case is based on samples irradiated with 20 MeV W^{6+} to a fluence of $8x10^{17}$ W/m^2, which corresponds to about 0.5 dpa. The modelled data set includes a set of samples exposed to plasma under identical conditions and degassed with different heating rates in order to elucidate binding energies and pre-exponential factors by the joint comparison of all simulated and measured TPD spectra. Using these parameters, we examined the dependence of the D inventory in damaged W samples as a function of fluence and temperature. To assess and determine parameters which are uncertain at very low hydrogen energies and affect the effective incoming hydrogen flux, i.e., reflection yield, stopping range and possible surface processes, we repeated the same experiments at a moderate sample bias of -100 V, which corresponds to 38 eV/D at an ion flux of $9x10^{19}$ D/m^{2}s, for further validation.

In our contribution, we present the details of the model and its underlying assumptions, and demonstrate that the model accurately predicts the fluence dependence of D depth profiles in damaged W under floating and biased plasma exposure conditions without any parameter adjustments. We also discuss shortcomings concerning the description of the temperature dependence of D retention in damaged W. Based on a parameter sensitivity study, we show how only one additional parameter can remedy the observed discrepancy of model and experiment. In the case presented here, it is necessary to vary the effective incident ion flux with the sample temperature. We also discuss possible physical explanations for the apparent temperature dependence of the effective ion flux.

[1*] K. Schmid et al., J. Nucl. Mater. 426 (2012) 247–253