The effect of a well-defined tungsten oxide layer on deuterium retention and release: a single crystal approach for macroscopic rate equations modeling

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Fusion fuel retention (trapping) and release (desorption) from plasma facing components are critical issues for ITER and for any future prototype reactors such as DEMO. Understanding fundamental mechanisms behind the retention of hydrogen isotopes in first wall and divertor materials is necessary. We developed an approach that couples dedicated experimental studies with modeling at all relevant scales, from microscopic elementary steps to macroscopic observables, in order to build a reliable and predictive fusion reactor walls model. In recent years, we have applied this integrated approach to ITER divertor material: polycrystalline tungsten. We were able to show that 10^{21} m^{-2} 250 eV deuterium (D) implanted in pristine W at 10^{16} $m^{-2}.s^{-1}$ diffuse 800 nm deep in the bulk and exhibits a dynamic retention at room temperature, with a release of half of the retained D within 48 hours, linked to a single desorption peak around 450 K. A Macroscopic Rate Equations (MRE) wall model initialized with Density Functional Theory (DFT) reproduced these experimental observables only if two rate-limiting steps were taken into account: detrapping from grain boundaries and detrapping through the native oxide layer [1]. However, quantitative agreement could not be achieved with such DFT-MRE model because of the ill-defined structure of the native oxide [2]. In this contribution, we focus on the influence of the native oxide on the D retention in tungsten.

A W(110) single crystal was used in a new UHV setup allowing *in situ* control of the oxide layer, structural characterization with low energy electron diffraction (LEED), deuterium ion implantation (250 eV/D) at a fluence of 3.10^{21} m^{-2} with 10^{18} $m^{-2}.s^{-1}$ and temperature programmed desorption (TPD). LEED showed that the native oxide is amorphous with inclusion of various crystallites. Annealing above 2000 K resulted in the removal of the native oxide and a truly clean W(110) with 1x1 reconstruction was obtained. 2x1 or 2x2 crystalline W oxide surfaces were grown by a combination of oxygen exposure and annealing in UHV. These W oxide have an oxygen surface coverage of ~0.5 monolayer (2x1 reconstruction) and ~0.75 monolayer (2x2).

Deuterium ion implantation resulted in an amorphization of the crystalline structure. However, the 2x1 and 2x2 reconstruction were recovered during the TPD evaluation of D retention. Differences in the shape of the TPD peak, with and without oxide, were observed that may be related to surface retrapping of implanted D. Most notably, by comparing D retention from ion implantation versus molecular exposure, we show that increasing surface order and increasing oxygen surface coverage both decreases D retention in the bulk of tungsten. Those well-defined crystalline structures make these results amenable to Density Functional Theory, which will allow the development of a DFT-MRE model of deuterium retention in W comparable, without approximation, to the present experiment observables.

[1] Hodille et al., Nuclear Fusion 57 (2017) 076019
[2] F. Ghiorghiu et al., Nucl. Instr. Meth. B, 461 (2019) 159