Hydrogen Isotope Exchange in Tungsten at Low Temperatures

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One possibility to reduce the tritium inventory of plasma-facing tungsten in future nuclear fusion reactors prior to opening the vacuum vessel is to perform hydrogen isotope exchange [1]. In this process a radioactive tritium (T) atom retained in a trap is replaced by a non-radioactive deuterium (D) or protium (H). Despite the extensive investigation of hydrogen isotope exchange in tungsten the underlying microscopic exchange mechanism remains unclear. Most of the available models consider the exchange empirically by the introduction of exchange cross sections or probabilities. A widely used microscopic model for hydrogen trapping in tungsten, termed classical model, assumes single occupancy of traps with hydrogen atoms and a fixed de-trapping energy depending on the trap type [2]. This model can explain the observed hydrogen isotope exchange only in very special cases and fails when the temperature is too low to allow thermal release of hydrogen atoms from the traps. In contrast to that, the recently developed fill-level model [3], which assumes multiple occupancy of traps and a de-trapping energy that decreases with increasing trap occupancy, is able to explain hydrogen isotope exchange on a microscopic scale also at low temperatures.
In order to test the fill-level model the exchange of D by H in tungsten is investigated in-situ in dedicated experiments with nuclear reaction analysis and mass spectrometry at low temperatures ranging from 150 to 290 K. In the first experiment the isotope exchange is investigated at 150 K for different D inventories prior to the exchange. The results show that a certain critical H fluence needs to be implanted before a decrease of the D inventory is observed. Furthermore, the lower the initial D inventory the larger the required critical H fluence. In addition, the decrease of the D inventory, once the critical H fluence is exceeded, is independent of the initial D inventory. In a second experiment the exchange of a pre-defined D inventory at different temperatures is studied. Also in this scenario, a critical H fluence is observed, which decreases as the exchange temperature increases. Furthermore, the decrease of the D inventory is stronger for higher exchange temperatures.
Finally, the experiments are simulated with the diffusion-trapping code TESSIM-X [3] in which the classical as well as the fill-level model is implemented. The observed dependences of the isotopic exchange on the initial D inventory and on the exchange temperature can be very well described with the fill-level model, whereas the classical model fails to reproduce the experimental results. However, since the exchange at low temperatures takes predominantly place within the implantation zone, kinetic de-trapping of D by energetic H cannot be neglected. When accounting for this effect in the simulations, also the classical model can describe the observed isotope exchange. This implies that an ensemble of classical traps with kinetic de-trapping behaves similar to a fill-level trap.

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[2] A. H. M. Krom et al., Metall. Mater. Trans. B 1475-1482 (2000) 31
[3] K. Schmid et al., J. Appl. Phys. 134901 (2014) 116