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Database for modelling of D transport and accumulation in W-based and Fe-based materials for ITER and DEMO

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To model hydrogen isotope migration and inventory in a metal under ion irradiation, rate equations are used. The diffusivity, solubility, surface barrier, reflection and sputtering coefficients, mean ion range, and binding energies of deuterium (D) with different types of defects are input parameters in the rate equations. Such parameters can be defined by ab initio calculations by DFT or MD or TRIM code and can be validated by comparison with experiment. TDS experiments are usually performed to derive de-trapping energies and recombination coefficient of D and permeation experiments to derive the diffusivity and solubility. D concentration in defects up to 10 microns can be measured by 3He nuclear reaction analysis, NRA. Defect characterization in materials is carried out by state-of-the-art experimental methods (STEM, PALS, EBSD, FIB-APT, etc.) before and after irradiation. In this contribution, the parameters of deuterium-defect interaction for W-based and Fe-based materials will be critically reviewed. The difference between speculative and reliable data and the interpretation of the experimental results will be shown.

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