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Modelling of hydrogen trapping, diffusion and permeation in tokamak

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Fuel retention and release from tungsten (W) Plasma Facing Components (PFCs) are key issues in the development of fusion as an energy source. Due to safety issues, a strict 700 g inventory tritium limit is required in the ITER vessel material. Moreover, the inventory of hydrogen isotopes (HIs) and their release back into the plasma can jeopardize its control due to too high radiated power at the edge. Furthermore, tritium permeation through PFC can lead to tritium spreading into the cooling loops. All of these phenomena must be efficiently predicted to allow safe and reliable tokamak operation. Thermo-kinetic models using macroscopic rate equations (MRE) are commonly used in that sense. If well validated by experimental comparisons, these models can predict fuel retention, particle recycling during plasma operation and hydrogen permeation through PFCs.

Here, the development of the MRE code MHIMS (Migration of Hydrogens Isotopes in MaterialS) will be reported. Then the finite element (FE) extension of such thermo-kinetic model will be described. It is used to follow the HIs behavior in complex 3D geometry and examples will be presented. Finally, the influence of helium (He) loading on the HIs inventory in W will be depicted with a preliminary modelling explanation.

MHIMS is a 1D MRE model where HIs inventory in W materials is split into two populations, a mobile and a trapped one. It has been validated through well-defined experiments and the strategy we have followed for this will be presented. Different free parameters are used to reproduce experiments that can be determined either by theoretical or experimental approaches. As an example, the diffusion coefficient of mobile species was derived from Density Functional Theory (DFT) [Fernandez-2015]. DFT also provides detrapping energies to be compared to the simulation results of experiments [Fernandez-2015]. Other parameters are extracted from laboratory experiments where a W sample is loaded with hydrogen (ions, atoms or gas). The hydrogen profiles in the material are measured by ion beam methods such as nuclear reaction analysis (NRA). Then Thermo-Desorption Spectrometry (TDS) is performed where HIs desorption rates are recorded during a linear temperature increase. In these TDS measurements, peaks appear at certain temperatures related to the HIs (de)trapping processes. MHIMS parameters are adjusted to reproduce these experiments.

Relevant parameters for trapping of HIs are determined [Hodille-2015] from HIs plasma loaded annealed polycrystalline tungsten. By comparison with TDS measurements, three types of traps are found: two intrinsic traps (detrapping energy of 0.87 eV and 1.00 eV) and one extrinsic trap created by ion irradiation (detrapping energy of 1.50 eV) for which the physical origin is supported by a DFT+thermodynamical model [Ferro-2018]. With the determined detrapping energies, HIs outgassing at room temperature is also well predicted.

Successful simulations of deuterium (D) retention in W ion irradiated polycrystalline tungsten following D atoms exposure at 500 K and 600 K are obtained thanks to an evolution of MHIMS. Bombardment of W samples by high energetic W ions mimics neutron irradiation. To be able to describe the exposure to D atoms, surface processes are implemented in MHIMS [Hodille-2017]. The TDS data are reproduced with three bulk-detrapping energies: 1.65 eV, 1.85 eV and 2.06 eV, in addition to the intrinsic detrapping energies known for undamaged tungsten.

Deuterium retention is then measured in tungsten samples simultaneously irradiated by W ions and D atoms at different temperatures [Markelj-2017]. Higher D concentrations are found in that case compared to sequential damaging and D atoms exposure. The observations are explained by the stabilization of defects that are occupied by D atoms. In order to model such a behavior, a novel displacement damage creation and stabilization model is introduced into the MHIMS code [Pečovnik-2020]. With this upgrade, the measured D depth profiles and TDS data are reproduced.

In order to simulate HIs behavior in thermally loaded structures in a Tokamak, full 2D finite element models are developed. For example, the 2D behavior of HIs retention in ITER monoblocks is studied using the code FESTIM (Finite Element Simulation of Tritium In Materials) [Delaporte-2019]. FESTIM is based on the same equations than the MHIMS 1D code and is validated by reproducing experimental laboratory data. Following relevant plasma scenarios, both transient heat transfer and HIs diffusion are simulated in order to assess HIs retention and permeation in monoblocks. It is shown that, after 100 ITER plasmas, tritium is localized in tungsten near the cooling channel. Tritium reaches the cooling channel after 24 ITER plasmas. Using 1D simulations, a relative difference of 25 % is observed compared to 2D simulations.

Another approach which in addition accounts for mechanical fields is implemented in the 3DS Abaqus software [Benannounne-2019]. The model is used to simulate the tritium diffusion and trapping in the ITER upper plug. It is shown that the thermal field heterogeneities observed in such components induces heterogeneous mechanical fields (due to the thermal expansion), which might affect, in return, the HIs transport through the induced hydrostatic pressure.

Finally, the impact of helium (He) plasma exposure on HIs trapping in PFC is investigated [Ialovega-2020]. TEM observation show that the size of the He bubbles increases with high-temperature cycling. In correlation, HIs trapping in the material is changing with a decreasing TDS peak temperature and a local increase in HIs retention. These behaviors are attributed to the evolution of the microstructure related to He bubbles. Preliminary Object Kinetic Monte Carlo simulations are confirming this hypothesis.

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