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Combined experimental and theoretical studies of the retention and permeation of hydrogen isotopes in fusion-relevant materials

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We present an overview of experimental facilities available at UKAEA-CCFE, as well as modelling studies that will be used in the course of the CRP. Hydrogen isotope ion exposure facility together with thermal desorption spectroscopy apparatus are already used at UKAEA to study deuterium retention in plasma-facing materials, such as Eurofer steel, Fe-Cr alloys [1], tungsten [2], and molybdenum. In the course of Tritium Retention in Controlled and Evolving Microstructure (TRiCEM) enabling research project, a collaboration has been established with several European research laboratories, that allowed us to perform self-ion irradiation of samples (University of Helsinki, Finland) and post-exposure characterization using SIMS (VTT, Espoo, Finland), TEM (CEA, Université Paris-Saclay, France), and PAS analysis (CEMHTI/CNRS, Université d'Orléans, France). This collaboration will be continued during the CRP.

Modelling efforts will be along two lines. On a small scale, similarity in saturation of vacancy content as function of damage, as observed in tungsten [2] and theoretically found by Derlet and Dudarev [3], will be investigated further. Parameters of tritium capture by defects, such as number of atoms and the depth of potential well, will be studied in ab initio and molecular dynamics calculations, as already done for dislocation loops in tungsten [4]. On a larger scale, tritium transport will be modelled under conditions of elastic stress field and temperature gradients.

1. A. Hollingsworth et al., Nucl. Fusion 60, 016024 (2020).
2. A. Hollingsworth et al., Deuterium retention and positron annihilation spectroscopy of self-ion irradiated tungsten, J. Nucl. Mater., under review.
3. P.M. Derlet and S.L. Dudarev, Phys. Rev. Materials 4, 023605 (2020).
4. A. De Backer et al., Nucl. Fusion 58, 016006 (2018).

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