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Multi-scale modelling of hydrogen isotopes retention and diffusion in highly irradiated materials

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A fundamental description of gas transport and retention in plasma-facing materials is crucial for tritium inventory modelling. During future reactor operations, the material microstructure is expected to evolve and reveal defects which act as "traps"for diffusing gas atoms, thereby compromising material performance. The classical formalism for gas diffusion and trapping is given by the McNabb-Foster equation [1] and Oriani equilibrium condition [2] to describe the reduction in diffusivity in the presence of traps. This "effective" diffusivity was initially proposed for single-occupancy traps under a *dynamic equilibrium*, where trapping and detrapping rates are equal.

In this work, we have developed a multi-gas, multi-trap, multi-occupancy and multi-dynamic transport code 'Palioxis'to bridge the gap between microscopic first principles and macroscopic partial differential equation approaches for modelling the diffusivity under irradiated conditions. We calculate the effective diffusivities of hydrogen isotopes in vanadium, tungsten and iron, as a function of homogenous vacancy concentration and gas concentration. In tungsten, the diffusivity monotonically increases with increasing hydrogen/gas content. However, a small drop in diffusivity is identified in vanadium and iron when gas and vacancy concentrations are comparable. The difference in behaviour between the elements is traced back to the difference in incremental binding energy of the *n*th hydrogen to an (*n*-1) vacancy complex. We validate the results from Palioxis by directly comparing effective diffusivities to those from molecular dynamics simulations performed with classical and machine-learning interatomic potentials.

[1] A. McNabb, P. Foster *Trans. Metall. Soc. AIME* **227** (1963)
[2] R. Oriani *Acta Metall.* **18** (1970)

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