Contribution ID: **13** Type: **contributed**

Microstructure impact on tritium retention and permeation in tungsten/oxide interface from first-principles based phase field modelling

Monday 26 May 2025 12:55 (20 minutes)

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Tungsten is a promising plasma-facing material for future fusion power plants owing to several favourable properties, including exceptionally high melting temperature, and excellent strength at high temperatures. However, lattice defects or "traps"created under fusion conditions in structural materials by 14.1 MeV neutrons from deuterium-tritium (D-T) fusion can increase the total HI retention in W by several orders of magnitude compared with unirradiated W. Moreover, due to its affinity for oxygen, W readily forms a natural oxide film on its surface at ambient temperature. This oxide layer, which may thicken under fusion device operating conditions on the "dark" side, or during maintenance, will critically influence HI uptake, T retention in, and release of T. Minimizing the loss of tritium through the exterior sides of a fusion device makes it imperative to have a better understanding of tritium solubility and diffusion in the sequence of defected WOx phases on W tile surfaces. A fundamental understanding of tritium permeation and retention behaviour in fusion materials components is essential for efficient tritium recovery, waste classification and performance of in-vessel materials under neutron irradiation. There is little literature investigating the detritiation of tungsten under these fusion-specific conditions.

In this work, the current results of an ongoing multiphysics investigation of the properties and microstructure of tungsten and its oxides relevant to tritium retention and transport, which is being undertaken for the UKAEA. A multi-scale materials modelling approach using first principles calculations combined with the machine learning potential developments and phase field simulation tools have been brought to bear on W oxidation and detritiation behaviour to provide mechanistic insights into key trends and input values for microstructural simulations. Diffusion of tritium in WO3 has been found to be like that in bulk W while diffusion of tritium is significantly slower in WO2 [1]. W oxide morphology, metal/oxide interface topology, and oxidation kinetics were qualitatively predicted successfully. Our work demonstrated that these characteristics of W oxidation are principally dictated by the interaction of phase nucleation, grain boundary diffusion and the emerging stress field. Tritium transport and prospects for efficient tritium recovery were shown potentially to depend on crack nucleation and growth processes in the W oxidation film, and on the dynamic metastability of a persistent WO2 -rich layer within the film. The results demonstrated a promising computational basis for informing the relative efficacy of various possible post-irradiation W tile handling scenarios bearing on tritium recovery.

[1M. Christensen et al., Materials and Energy, 38 (2024) 101611

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Session Classification: contributed