Contribution ID: **41** Type: **not specified**

# Modeling and Experimental Investigation of Hydrogen Permeation in Fusion Materials

*Monday, 23 November 2020 14:40 (20 minutes)*

The recycling of hydrogen isotopes in the plasma (fuel) is self-regulated through processes involving near-surface diffusion, trapping, and gas bubble formation, coupled to the ionization that results from interactions with the plasma. The multitude of time and length scales controlling material evolution and device performance requires the development not only of detailed physics models and computational strategies at each of these scales, but also experimental validation. Similarly, the permeation of tritium through first wall structural materials and the components within the breeding blanket is critically important for assessing the tritium breeding ratio and sustainability of the fusion fuel cycle, and involve a hierarchical, multiscale set of phenomena.

This project seeks to integrate computational simulations of materials evolution under fusion relevant exposure conditions with microstructural characterization and focused mechanism-based experiments to provide improved understanding of fusion materials behavior. This program addresses several critical questions associated with PFC and first wall/blanket materials performance in materials systems ranging from model alloys to tungsten-based PFC/divertor materials, in addition to iron-based first wall and blanket structural materials and a fundamental investigation of radiation effects in model alloys, and the impact on hydrogen permeation and trapping inventory.

The first year will focus on expanding our experimental measurements of deuterium permeation through tungsten and ferritic-martensitic alloys as a function of initial microstructure, to include different grain sizes, radiation damage and helium bubble distributions. These experimental studies will also involve different microstructure characterization tehcniques, and be complemented by multiscale modeling studies, ranging from ab initio density functional theory assessments of hydrogen diffusion and interaction with microstructural features, large-scale molecular dynamics simulations of hydrogen permeation and continuum level reaction-diffusion cluster dynamics modeling of the permeation and thermal desorption experiments.

**Primary author:** Prof. WIRTH, Brian (University of Tennessee)

**Co-authors:** Mr CHEN, Ze (University of Tennessee); Ms GARCIA, Wendy (University of Tennessee); Dr HU, Xunxiang (Oak Ridge National Laboratory); Dr HUANG, Gui-yang; Dr LASA, Ane (University of Tennessee); Dr YANG, Li (University of Tennessee)

**Presenter:** Prof. WIRTH, Brian (University of Tennessee)

**Session Classification:** Atomistic modelling I