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Multiscale Modelling of Hydrogen Retention in High Dose Irradiated Microstructures

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Component-scale predictive models for how hydrogen isotopes interact with, and are retained by, irradiation-induced defects are required to inform design decisions in materials for fusion power. This is a multiscale materials modelling challenge, with a conceptual gap between electronic structure calculations on one hand, which provide high accuracy estimations of idealised elemental defect structures and binding, and partial differential equations on the other, which provide the long timescale evolution behaviour. This gap is due to the complexity of realistic irradiation microstructures.

We have developed and validated an interatomic potential suitable for large-scale molecular dynamics simulations in tungsten with hydrogen isotopes present[1], and used it to explore how defects respond to decoration by deuterium and tritium. In parallel, we have refined and simplified the mathematical formalism required to model generic gas-retention by complex defects, and developed a library of code providing a simple, flexible framework for modelling tritium retention in complex microstructures integrated into MOOSE.

In this talk I will describe recent work at UKAEA generating hydrogen isotope-decorated high-dose microstructures in tungsten[2,3], and validating atomistic and finite element simulations[4] against laboratory-scale experiments.

References:
[1] D.R. Mason, D. Nguyen-Manh et al, J. Phys. Cond. Matt. 35:495901 (2023)
[2] M. Boleininger, D.R. Mason et al, Sci. Rep. 13:1684 (2023)
[3] D.R. Mason, F. Granberg, et al, Phys. Rev. Mater 5:095403 (2021)
[4] https://github.com/aurora-multiphysics/achlys

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