

Dislocations Informed Crystal Plasticity Modelling of Hydrides in Zr-alloy Fuel Cladding Materials

This project will focus on developing dislocation-scale informed rules for representation of Zr-alloy hydride behaviour in Crystal Plasticity (CP) models for larger scale simulation of irradiated microstructures.

Discrete dislocation plasticity (DDP) models of irradiated material will be used and developed to inform representations of critical resolved shear stress and new flow rules that account for the effects of irradiation hardening due to dislocation-loop interactions, and subsequent softening caused by channel clearing; the nature of hardening in response to changing loop density, for example, will be identified from DDP modelling for use in CP, while other CP quantities may be informed by DDP. This will allow for more realistic predictions of plasticity and stress distributions around hydrides in irradiated material at the microstructural scale under realistic temperature and stress histories. Accurate prediction of the background stress, particularly under thermal cycling, is needed to predict hydrostatic stress evolution, hence hydrogen concentration for use in hydride nucleation criteria. Thermodynamic hydride precipitation rules will be developed in the project, which can be utilised at both the DDP and CP model scales.

Further work may be possible in utilising machine learning approaches trained by the CP models to capture broad microstructural parameter spaces, and/or the use of homogenisation techniques to capture the average effect of hydride populations without modelling them explicitly.