Study of the effect of the zirconium grain structure on hydride precipitation using phase field modeling

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In light water reactors, waterside corrosion of nuclear fuel cladding material results in the production of hydrogen, which is partially picked up by the cladding. Once the concentration of hydrogen reaches the solubility limit, hydride precipitation can occur. The hydride microstructure may consist of brittle nanoscale hydrides which aggregate into mesoscale hydrides. The mesoscale hydrides can affect the performance of the nuclear cladding both during normal operation and during dry storage. The effect of the hydrides on cladding mechanical properties depends on hydride morphology and orientation, which are in turn dependent on material crystallographic texture, and on the thermomechanical history experienced by the material.

In particular, during drying operations as a prelude to dry storage, the cooling from high temperature under stress can cause hydride reorientation. While mesoscale hydrides are usually elongated along the circumferential direction of the cladding, they can precipitate radially when cooled under stress, which facilitates crack propagation through the cladding thickness when subjected to a hoop stress. Thus, to ensure safe handling of spent fuel it is necessary to develop a quantitative model of hydride morphology development. Since mesoscale hydrides are typically much longer than the zirconium grains, understanding how nanoscale hydrides aggregate across grain boundaries is crucial to understanding the mesoscale hydride morphology.

In this study, a quantitative phase field model is applied to the zirconium hydride system to investigate the effect of grain-to-grain misorientations and of the presence grain boundaries on the formation of mesoscale hydride microstructures starting from nanoscale hydride precipitation. The model predicts that upon reaching a grain boundary a growing hydride grows into the neighboring grain respecting the orientation relationship with the new grain, rather than simply growing straight. Moreover, the presence of an elongated nanoscale hydride in one grain influences the hydride nucleation in a neighboring grain, leading to a preferential stacking of nanoscale hydrides across grain boundaries.