

Elastoplastic Phase Field Model for Time-dependent Hydrogen Diffusion, Hydride (and Blister) Formation and Fracture Initiation in Zirconium

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Summary

Zirconium and its alloys are key structural materials used in the nuclear power industry. In service, these metals are susceptible to a slow corrosion process that leads to a gradual pickup of hydrogen impurities from the environment. It is well known that hydrogen impurity will be attracted to stress concentrators such as notch and crack tips. At a certain hydrogen level, a complicated pattern of hydride precipitates can develop around these stress concentrators. Because of the brittleness of these hydrides, the original strength of the alloys can be reduced by orders of magnitude, and the fracture through these hydrides may occur. It is believed that critical conditions for the initiation of fractures at hydrides are controlled by the morphology and microstructure of hydride precipitates. In recent years by using a linear elastic approach, the author's research team has simulated the morphological and microstructural evolution of hydride precipitation in single and polycrystalline zirconium under uniform and non-uniform stress fields. The methodology was based on the principles of the Ginzburg-Landau kinetic phase-field theory coupled with Cahn-Hilliard diffusion dynamics, the method that has enjoyed much success in recent years. However, it is well known that plastic deformation will occur during hydride formation in zirconium alloys, and that plasticity around flaw tips may also play an important role during hydride fracture. The objective of this work is to incorporate plastic deformation into the phase field model and to develop computational methodologies to predict the realistic 3-D morphological evolution of hydride precipitates around notch and crack tips, hydride blister formation, and ultimately to predict fracture initiation at hydrides in zirconium.

