Quantitative, Elastoplastic Phase Field Model for Microstructural Evolution during Hydride Precipitation in Zirconium under Stress and Temperature Gradients

San-Qiang Shi

Department of Mechanical Engineering, The Hong Kong Polytechnic University
Hung Hom, Kowloon, Hong Kong, China
mmsqshi@polyu.edu.hk
Homepage: www.polyu.edu.hk/me/files/sqsscv.pdf

Abstract

Zirconium and its alloys 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 migrate under stress and/or temperature gradients. At a certain hydrogen level, a complicated pattern of hydride precipitates can develop, and hydride precipitation involves a large volume expansion more than 16%, which results in elastoplastic deformation of the alloy. 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, the author's research team has developed a phase-field scheme to simulate the morphological and microstructural evolution of hydride precipitation in single and polycrystalline zirconium under uniform and non-uniform stress and temperature fields. Recent effort was devoted to develop a quantitative model. The model takes into account crystallographic variants of hydrides, interfacial energy between hydride and matrix, interfacial energy between hydrides, elastoplastic hydride precipitation and interaction with externally applied stress and/or temperature field. The model is fully quantitative in real time and real length scale, and simulation results were compared with limited experimental data available in the literature with a reasonable agreement. This work was supported by grants from Research Grants Council of Hong Kong (PolyU 5267/10E) and the Natural Science Foundation of China (No.51271157).