

Quantitative, elastoplastic phase-field model for microstructural evolution in solids under stress and temperature gradients

S.Q. Shi^{1,2}

¹Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong, China

²The Hong Kong Polytechnic University Shenzhen Research Institute, Shenzhen, China

mmsqshi@polyu.edu.hk

Abstract

Quantitative prediction of three-dimensional microstructure evolution during phase transformation in solids is often very challenging, especially when stress, composition and temperature gradients are present, together with plastic deformation. This paper takes hydride precipitation in zirconium alloys and void growth in irradiated metals as examples and shows how it could be done in nano-, micro, meso- and macro-scales within phase-field scheme. 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 for hydride precipitation and void growth. The model for hydrides takes into account crystallographic variants of hydrides, interfacial energy between hydride and matrix, interfacial energy between different hydrides, elastoplastic hydride precipitation and interaction with externally applied stress and/or temperature field. The model for hydrides and for void are fully quantitative in real time and real length scale, and simulation results were compared with limited experimental data available in the literature with reasonable agreement. However, some numerical and physical issues remain to be solved. 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).

Keywords: Quantitative Computer Modeling, Phase-field method, Stress, Temperature Gradient

References

- Shi, S.Q. and Xiao, Z.H. (2015) A quantitative phase field model for hydride precipitation in zirconium alloys: Part I. Development of quantitative free energy functional, *Journal of Nuclear Materials* **459**, 323–329.
- Xiao, Z.H., Hao, M.J., Guo, X.H., Tang, G.Y. and Shi, S.Q. (2015) A quantitative phase field model for hydride precipitation in zirconium alloys: Part II. Modeling of temperature dependent hydride precipitation, *Journal of Nuclear Materials* **459**, 330–338.
- Xiao, Z.H., Semenov, A.A., Woo, C.H. and Shi, S.Q. (2013) Single void dynamics in phase field modeling, *Journal of Nuclear Materials* **439**, 25–32.