Microstructure-based modeling of nuclear materials in extreme conditions

Abstract: Nuclear energy is an essential part of our energy sustainability. The reliability and economics of nuclear energy is strongly limited by the performance of fuels and materials, which are subject to significant degradation caused by the extreme reactor environments. It is critically needed to predict the degradation rates for the life-time extension of current reactors and for the development of future nuclear technologies. While the degradation effects are usually observed at the engineering scale, their causes originate from the atomic scale. The huge gaps in time and length scales make it a grand challenge to uncover the degradation mechanisms for predicting the degradation rates. In this talk, a microstructure-based, multiscale modeling and simulation approach will be presented for materials behavior in extreme conditions. It focuses on the evolving microstructure to simulate the degradation, and the structure-property correlations to predict the transient properties. It is closely coupled with experiments and theories for in-depth understanding and for true predictivity. As a demonstration, two detailed examples, void superlattice formation under irradiation in bcc metals and hydride nucleation in Zr-based alloys, will be presented. Currently, this approach is being applied to a list of degradation phenomena in fuels and claddings of light water reactors. It is expected to make more significant impact for fuels and materials used in future reactors.

Biography: Dr. Yongfeng Zhang is currently a staff scientist at Idaho National Laboratory, INL. He leads the Computational Microstructure Science group in the Fuel Modelling and Simulation Department. He has served as the PI of multiple Department of Energy (DOE) program work packages and INL laboratory directed research & development (LDRD) projects. He is also a co-PI of a core program and an Energy Frontier Research Center supported by DOE Office of Science. Dr. Zhang obtained his PhD in Mechanical Engineering from Rensselaer Polytechnic Institute in 2009 and joined INL after that. His research focuses on microstructural level modeling of materials behavior in extreme conditions, including high temperature, stress, irradiation and corrosive media. The topic areas including radiation effects, mechanical deformation, and property degradation. He has authored and co-authored over 50 peer-reviewed journal publications and delivered over ten invited talks at conferences and university seminars. He has been recognized multiple times at INL, including the Laboratory Director’s Award for Leadership for 2016.

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