Phase-Field Simulation of Void and Fission-Gas Bubble Evolution in Irradiated Polycrystalline Materials

Paul C. Millett[1], Anter El-Azab[2], Michael Tonks[1], Srujan Rokkam[2], Dieter Wolf[1]

[1] *Nuclear Fuels and Materials, Idaho National Laboratory, Idaho Falls, ID 83415, USA*
[2] *Dept. of Scientific Computing, Florida State University, Tallahassee, FL 32310, USA*

The interactive evolution of both polycrystalline microstructure and irradiation-induced defects such as voids and fission gas-filled bubbles in nuclear fuels and structural alloys is complex and critically important to the long-term performance of fission reactors. Here, the phase-field technique is used to model the evolution of multiple point-defect species (vacancies, self-interstitials, and gas atoms), generated randomly in space and time to represent collision cascade events, thus allowing spatially-resolved simulations of void and gas bubble nucleation and growth both within grain interiors and at grain boundary interfaces (which are shown to be heterogeneous nucleation sites). Illustrative results including the formation of void denuded zones and void peak zones adjacent to grain boundaries, and the interlinkage of intergranular gas bubbles leading to fission gas release will be presented. This work was supported by the DOE-BES Computational Materials Science Network (CMSN).