In Situ Ion Irradiation to Add Irradiation Assisted Grain Growth to the MARMOT tool

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ABSTRACT: In the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, the MARMOT mesoscale fuel performance tool is used to inform the development of mechanistic materials models for the BISON fuel performance tool. The grain size of the fuel has a large impact on its performance, directly impacting heat conduction, fission gas release, creep, and fracture. Thus, atomistic and mesoscale MARMOT simulations have been used to investigate grain boundary migration and grain growth in UO$_2$. Figure 1 shows an example of one such grain growth simulation in MARMOT. However, the current grain growth models in MARMOT only consider grain growth kinetics of fresh, unirradiated fuel. This proposal is to experimentally study and ultimately implement irradiation effects on grain growth of UO$_2$ into MARMOT.

This work will proceed with coincident and synergistic efforts of experiment and simulation. In-situ transmission electron microscope (TEM) experiments will be performed at Argonne National Laboratory to study grain growth in both isothermal annealing conditions and ion irradiation conditions. The data obtained from these experiments will be used to quantify the kinetics of grain growth under these conditions, inform the physical mechanisms for implementation into MARMOT, and serve as validation data for MARMOT simulations. Irradiation effects of grain growth will be added to MARMOT and the improved tool will be used to assess the impact of the irradiation effects on light water reactor (LWR) fuel. The most important deliverable of this project will be the expanded capabilities and validation of the MARMOT tool to advance the agenda of the NEAMS program, in the form of grain growth due to irradiation added to MARMOT, and data for validation of in-situ isothermal annealing and irradiation grain growth. In addition, journal publications and conference presentations divulging the experimental results, model development, and simulations are expected. Finally, deliverables in the most basic sense will include periodic reports the NEUP and these will be provided at the times and frequency requested.