A Coupled Experimental and Simulation Approach to Investigate the Impact of Grain Growth, Amorphization, and Grain Subdivision in Accident Tolerant U3Si2 Light Water Reactor Fuel

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ABSTRACT:

The low thermal conductivity of UO_2 results in high fuel rod temperatures, which are extremely dangerous in accident conditions. Triuranium disilicide (U_3Si_2) is being considered as an alternative accident tolerant fuel (ATF) due to its higher thermal conductivity. However, there is uncertainty in its use due to a lack of irradiation data at light water reactor (LWR) conditions. While the Fuel Cycle Research and Development (FCRD) and Nuclear Energy Advanced Modeling and Simulation (NEAMS) programs are aggressively investigating this fuel, there are important behaviors that they do not have the resources to investigate. In this project we propose to use an integrated experimental and simulation approach to answer two significant questions pertaining to U_3Si_2 that are not being investigated by NEAMS or FCRD:

1) Will grain growth in the hotter portions of the fuel significantly impact U_3Si_2 LWR fuel behavior?
2) Under what conditions do grain subdivision and amorphization occur in U_3Si_2 and will either occur at LWR conditions?

The integrated approach that we will use to answer these two questions has been broken into three tasks, where the first addresses grain growth, the second grain subdivision, and the last grain amorphization, as shown in Fig. 1. The first task will be accomplished by using bicrystal and polycrystal experiments along with atomistic molecular dynamics (MD) simulations to determine typical GB mobilities and energies for U_3Si_2. These results will be used in simulations with the MARMOT mesoscale fuel performance tool to quantify grain growth that will occur in the fuel and to implement a grain growth model for U_3Si_2 in BISON. To answer our question regarding grain subdivision, we will determine temperature and dose thresholds for subdivision in U_3Si_2 using both in situ ion irradiation experiments and comparisons between the energies in subdivided and non-subdivided structures using free energy functions in MARMOT. Ion irradiation will also be employed at various temperatures in task three to determine the necessary conditions for amorphization. A phase field model of amorphization will be developed in MARMOT, informed by MD simulations, to assist in the investigation of amorphization.

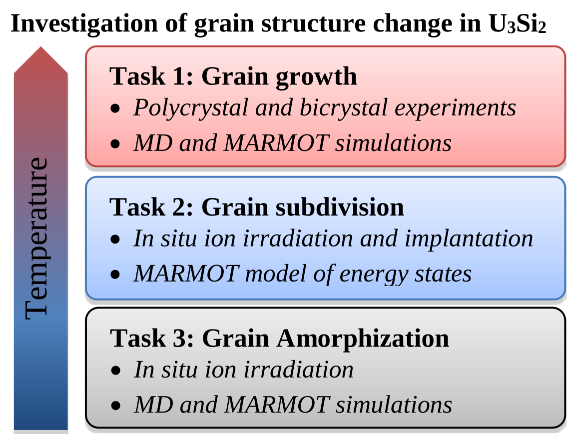

Figure 1: A schematic diagram of the proposed integrated experiment and modeling approach to investigate grain growth, amorphization, and grain subdivision in U_3Si_2.