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Fuel Performance Experiments on the Atomistic Level, Studying Fuel Through Engineering Single Crystal UO_2

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ABSTRACT

The single-crystal UO2 program is designed to build custom-engineered single-crystal UO2 samples for determining the basic physical properties of UO2 fuel. By producing custom-engineered single crystals, phenomena such as fission-product migration, fuel-cladding interactions, grain formations, grain propagation, and heat transfer across grains can be studied in a controlled environment. These studies combine state-of-the-art fuels modeling with unprecedented accuracy and precision experiments in a highly ordered system. All of this work is in support of current and next-generation fuel types for atomistic to macroscopic scale modeling efforts. This project is aimed at determining many of these fundamental physical properties in support of the FC research and development (R&D) efforts.

Fuels performance today is being calculated on the atomistic level all the way up to the full core calculations using sophisticated simulation computer codes bridging the gap between the microscopic and macroscopic. It is proposed to measure with unprecedented precision and accuracy, atomistic properties, fission-product behavior, and grain mobility of current and new fuel designs as well as cladding and structural materials in reactor-based environments through custom-grown engineered single-crystal uranium oxide samples.

The number of parameters that exist when studying microscopic through atomistic phenomena in a fuel pellet are far too many to ascertain single effects from each separate component. Integral quantities can be obtained, but not on an atomistic or microscopic level. By producing engineered single uranium or other transuranic oxide and nitride crystals that focus in on a single materials parameter, single, separate effects tests can be conducted. With a host of single effects tests, a dataset of fuels performance studies can be created to help the modelers with phenomena they only have integral quantities for.

The main focus of this data campaign is on single-crystal heat diffusion and the effect on the crystalline structure and fission-product mobility of the UO2 pellet. It is proposed to develop the capability to measure these physical parameters, specifically temperature and pressure effects on engineered single-crystal fuels. These tests will require the development of a special nuclear fuel "oven" in which the coolant material, pressure, and temperature can be changed in real time. The proposed "oven" will provide a unique opportunity to obtain information on the temperature and pressure effects on single-crystal fuel samples in real time measuring heat propagation, thermal expansion, fission-product mobility, and grain formation and propagation. Quantifying these separate effects on defect migration will provide insight into the behavior of nuclear fuels. This custom-designed oven will provide "line of sight" so that microstructural data may be obtained in real time down to nanometer resolutions, providing valuable insight into the evolution of defects and fuel-sample deformation. Since temperature and pressure are only two of the parameters that affect nuclear fuel behavior, the proposed oven will be designed in such a way that it can be easily integrated into a comprehensive separate effects testing capability that in the future can include gamma and neutron irradiation capabilities.