Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)

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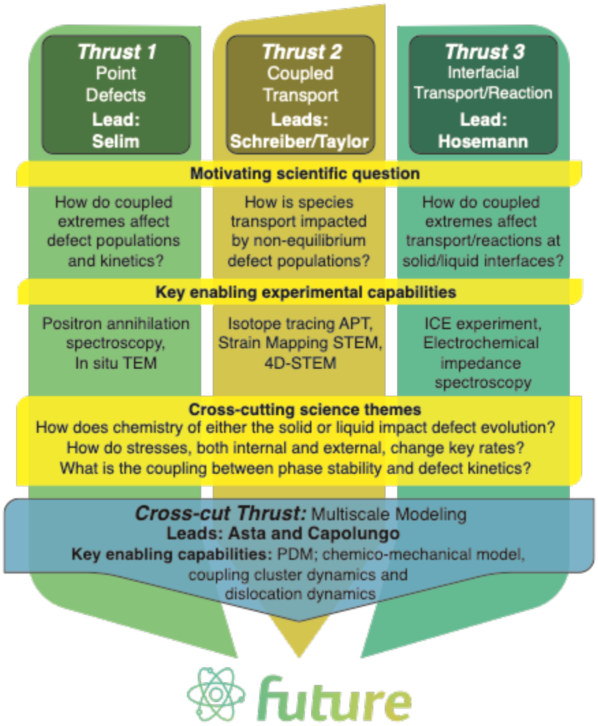
***Mission Statement**: To understand how the coupled extremes of irradiation and corrosion work in synergy to modify the evolution of materials by coupling experiments and modeling that target fundamental mechanisms.*

Nuclear reactor environments are some of the most hostile and extreme built by humans. A multitude of harsh conditions exist simultaneously, all acting in concert to degrade the performance of the materials. These extremes include irradiation, temperature, stress, and corrosion. Irradiation damage itself is one of the greatest materials science challenges as it is truly multiscale, spanning from subatomic effects at the femtosecond time scale to macroscopic consequences for reactor components as large as the pressure vessel on the time scale of decades. Coupling irradiation with other harsh environments such as corrosion leads to an immense scientific challenge requiring a multidisciplinary team. We have assembled such a team in FUTURE.

In FUTURE, we target the response of materials to a combined corrosive and irradiation environment at relevant conditions of temperature and stress. Corrosion is driven by mass transport to and from reactive surfaces, across interfaces, and/or through protective scale layers. At the same time, the transport of species in the bulk material can lead to materials degradation. As the corrosion front advances, particularly when a new phase is formed via, for example, oxidation, stresses may build up that affect transport, altering both defect concentrations and mobility. On the other hand, radiation changes the concentrations and nature of the rate determining defects. That is, the defects that define corrosive behavior under thermal conditions may be irrelevant under irradiation. All of these defects will couple with elemental species intrinsic to the material and coming from the corrosive medium. It is critical to understand the coupling of irradiation-induced defects with elemental species in a corrosive environment to predict the response of the material in these coupled extremes.

By combining modeling and experiment, FUTURE targets these fundamental mechanisms. Our experimental campaign, broken into three Thrusts, focuses on three fundamental questions underlying the response of materials to coupled irradiation and corrosion extremes: what is the nature of the defects produced by irradiation, how do those defects couple with the various elemental species in the material to change the local chemical composition, and how is transport across interfaces modified by irradiation. We are developing unique experimental capabilities that target these questions. In the case of point defect generation during irradiation, we complement in situ transmission electron microscopy (TEM) studies with positron annihilation spectroscopy (PAS) to understand the nature of irradiation-induced defects. TEM is a work-horse in irradiation studies and is able to characterize and quantify the nature of large defect aggregates. PAS compliments this capability by being able to quantify point defects, such as vacancies and small vacancy clusters. We are designing a PAS capability on LANL's existing ion beam lines to quantify these defects in situ as irradiation is happening, as opposed to typical studies in which defect content is quantified after the fact.

These studies are complemented by advanced microscopy characterization that examines how defects couple with elemental species in the material to modify overall evolution. In particular, we use advanced



4D microscopy techniques to examine how microstructural features interact with defects and alloying elements to modify transport pathways. Uniquely, we are using isotopic atom probe tomography (APT) to determine how species such as oxygen migrate through the microstructure. By using isotopic labels, we can determine those regions in which transport is enhanced most significantly.

Finally, we are targeting transport across the liquid/solid interface. We are using electrochemical impedance spectroscopy (EIS) to quantify key reaction rates at these interfaces. We are also expanding on a unique capability in which a material is exposed simultaneously to a coupled irradiation and corrosion environment. This irradiation-corrosion experiment (ICE) has been used to study liquid metal corrosion. We are expanding this capability to also target molten salt environments. This provides a direct and controlled experimental capability to understand how factors such as temperature and irradiation spectrum interact with the corrosive medium to modify the material properties.

All of this experimental activity is complemented by a cross-cutting modeling activity that aims to both elucidate the mechanisms observed in the experiments and develop a capability to predict the evolution of materials under these coupled extremes. The heart of this multi-scale effort is a new capability to be developed in FUTURE. This concurrent chemico-mechanical model, termed CD^3, combines cluster dynamics and dislocation dynamics to simulate the chemical evolution of a system in an evolving irradiated microstructure. This modeling framework enables predictions that account for the microstructural evolution induced by irradiation that can be directly compared and validated against the experimental studies conducted in Thrusts 1-3.

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