Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)
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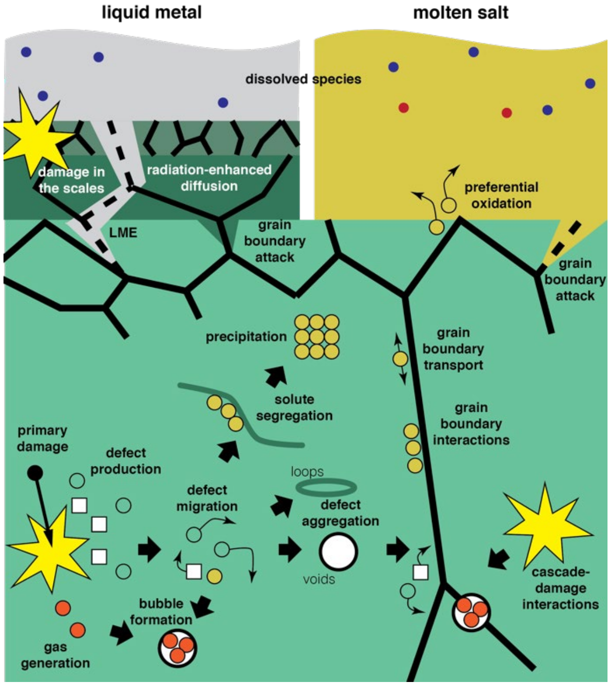
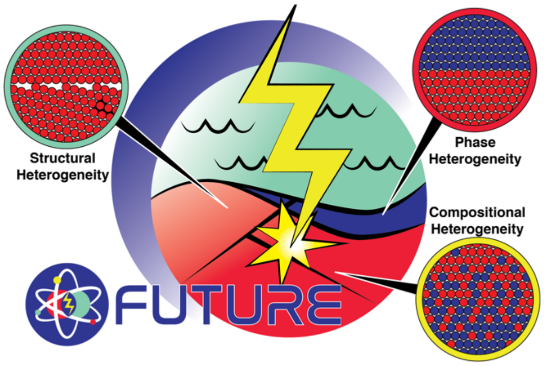
Mission Statement*: To understand how the coupled extremes of irradiation and corrosion work in synergy to modify the evolution of materials by coupling experiments and modeling that target fundamental mechanisms.*

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 that comprise the system. These extremes include irradiation, temperature, stress, and corrosion. Individually, irradiation damage and corrosion are two of the greatest materials science challenges as they are truly multiscale. For example, radiation effects span 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. Corrosion mechanisms differ depending on if the corrosive environment is a molten salt versus an oxygenated system that induces oxide formation. Coupling irradiation with corrosion leads to an immense scientific challenge requiring a multidisciplinary team, just as we have assembled such a team in FUTURE.



In FUTURE, we target the response of materials to a combined corrosive and irradiation environment. 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. Building on the success of the first phase of FUTURE, in this second phase we target materials heterogeneities. Real materials are characterized by heterogeneities – "disruptions of perfect order" – that often dictate their response to extreme conditions. These include structural heterogeneities such as grain boundaries and dislocations, phase heterogeneities in which multiple phases are present at once, and compositional heterogeneities where chemical species are distributed non-uniformly throughout the material. At the



same time, radiation damage and corrosion both induce new heterogeneities in the material, leading to a dynamic feedback between the response and structure. In FUTURE, we focus on these heterogeneities with the goal of understanding how they couple to radiation damage evolution and corrosion mechanisms to modify the response of the material to these combined extreme environments. This coupling leads to three hypotheses that guide the scientific research of FUTURE:

- The energy landscape for transport in compositionally-heterogeneous alloys and oxides alters the rate and prevailing mechanisms of corrosion and is, in turn, modified by irradiation.
- The thermokinetics of defect evolution and thus ongoing corrosion, thermally and under irradiation, differ in a multiphase vs. single phase material.
- The dynamics of transport that drive corrosion through extended defects and their networks are altered under irradiation.

Understanding how these heterogeneities impact the coupling between irradiation and corrosion requires a wide-range of expertise in radiation damage and corrosion science, unique modeling techniques, and integrated experimental facilities that can only come from a Center such as FUTURE. We have developed novel modeling and experimental capabilities to interrogate and understand this coupling. These include in-situ positron annihilation spectroscopy, where the positron beam is coincident with an ion beam to probe damage evolution in situ; the Irradiation-Corrosion Experiment, which provides the ability to subject a material to irradiation while also be exposed to a corrosive environment; buried isotope markers and atom probe tomography, to directly quantify radiation-enhanced diffusion; a cluster dynamics model of coupled irradiation and corrosion, accounting for the myriad of reactions that describe the interaction between radiation-induced defects and corrosion mechanisms; and a new multi-phase field model that predicts the morphological evolution of metallic alloys in a dealloying regime.

The goal of FUTURE is to reveal the fundamental factors dictating the evolution of materials under the coupled extremes of irradiation and corrosion with a goal of developing a predictive capability for these materials.

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