Energy Dissipation to Defect Evolution (EDDE)
EFRC Director: Yanwen Zhang
Lead Institution: Oak Ridge National Laboratory
Class: 2014 – 2020

***Mission Statement**: To understand how extreme chemical complexity can be exploited to control energy dissipation and defect evolution under equilibrium and non-equilibrium conditions and to guide the development of radiation-tolerant alloys with unique magnetic and thermal properties.*

Means of improving the performance of structural materials have been intensively investigated for many decades. Solid solution strengthening, traditionally achieved by alloying minor elements into pure metals or conventional alloys, is one of the most widely used methods to attain specific desirable properties, including radiation tolerance. It has long been recognized that alloys with specific compositions exhibit enhanced radiation resistance; however, it remains unclear how the atomic-level structure and chemistry affect defect formation and damage evolution during irradiation. This knowledge gap has been a roadblock to the development and implementation of future-generation energy technologies.

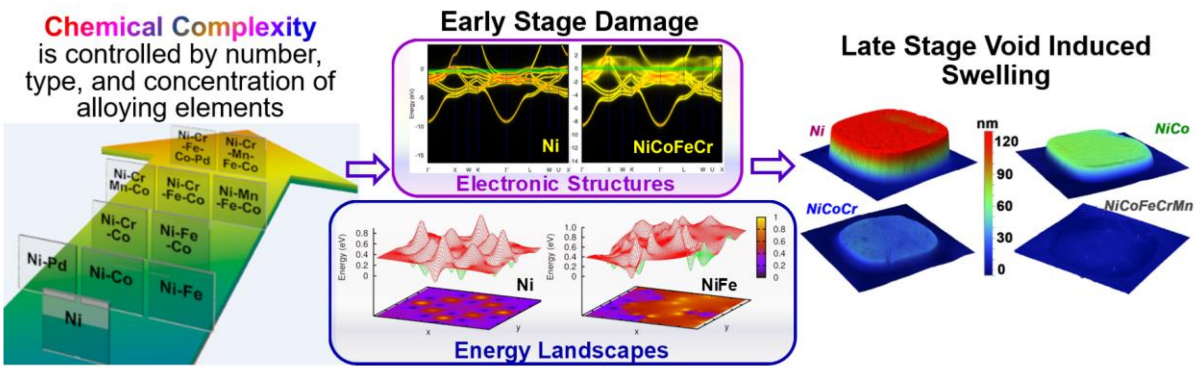

Fig. 1. EDDE aims to understand and tailor chemical complexity in model alloys (subset of SP-CSAs shown on left), which represents a powerful tool for dramatically modifying electronic and atomic properties (middle), and ultimately enhancing radiation tolerance (right) by reducing the rate of Energy Dissipation (Thrust 1) and controlling Defect Evolution (Thrust 2).

The predictive discovery and guided design of advanced materials with targeted functionalities will be key to enabling modern technologies, especially for future nuclear energy applications. A new class of alloys—Single–Phase Concentrated Solid–solution Alloys (SP-CSAs) composed of multiple elements, all at high concentrations—exhibit unexpected and exceptional properties, e.g., robust phase stability, ultrahigh low-temperature toughness, high-temperature strength, superparamagnetism, superconductivity, and importantly, suppressed irradiation-induced damage accumulation and void formation. In the EDDE Center, we hypothesize that by understanding and optimizing the chemical complexity both locally and globally in SP-CSAs (Fig. 1 left; Zhang, et al., *Current Opinion in Solid State and Materials Science* **2017**, 21, 221–237), energy dissipation and defect evolution can be tailored upon individual radiation events to encourage defect annealing within the picosecond time scale (Fig. 1 middle; Zhao, et al., *Physical Review Materials* **2018**, 2, 013602; Zhang, et al., *Nature Communications* **2015**, 6, 8736), and ultimately suppress damage accumulation under prolonged high-dose irradiation (Fig. 1 right; Lu, et al., *Nature Communications* **2016**, 7, 13564). We will understand and exploit the ability to tailor the chemical complexity of SP-SCAs, to thereby control energy dissipation via energy carriers that transport charge, heat, and spin (Fig. 1 middle top) and to control defect evolution resulting from kinetic energy transfer and mass transport during and after radiation events (Fig. 1 middle bottom), e.g., collision cascades and defect migration. The EDDE Center will study the extreme chemical complexity that arises from intrinsic elemental disorder in SP-CSAs to fundamentally understand an alloy's performance in extreme environments and reveal design principles for the predictive discovery and guided synthesis of new alloys with targeted functionalities, well beyond radiation tolerance.

EDDE's research is structured around two intertwined research Thrusts implicit in the Center's name: Energy Dissipation (Thrust 1) aims to understand the complex interactions among the energy carriers (electrons, phonons, and magnons) that dissipate elastic and inelastic energy deposited in a material; Defect Evolution (Thrust 2) aims to control the energy landscapes and tailor atomic transport processes to impact both defect production during collisional energy transfer in the femtosecond to picosecond time frame and damage evolution over longer time scales. The EDDE Center has extensive experience in growing high-quality, large, single crystals with targeted compositions; collaborative execution of well-defined irradiation experiments and microstructural characterization (including *in situ* ion beam analysis techniques, ultrafast science, and high-resolution microscopy/spectroscopy); world-leading theoretical and modeling expertise; and development of high-performance computer codes that extend the size and complexity of systems amenable for theory, modeling, and high-throughput discovery. The study of SP-CSAs through a combination of deep theoretical understanding, state-of-the-art computational approaches, and cutting-edge synthesis and experimental methods will enable us to elucidate the mechanisms controlling defect dynamics and irradiation performance of SP-CSAs based on fundamental energy scattering mechanisms. The synergy between the EDDE Center's team members within ORNL and with its partner institutions will allow EDDE research to capitalize on the team's outstanding strengths, thereby achieving rapid scientific advances.

The development and study of unique SP-CSAs in the EDDE Center have prompted new questions that challenge established theories and models currently applicable to conventional (dilute) alloys. Our overarching goal is to provide comprehensive knowledge of how the chemical complexity of SP-CSAs manifests and ultimately controls energy dissipation and defect evolution under extreme conditions. The success of the EDDE Center will provide a foundation that will enable breakthroughs in the design of revolutionary new materials and will present unforeseen opportunities for materials discovery.

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