# Machine Learning on High-Throughput Databases of Irradiation Response and Corrosion Properties of Selected Compositionally Complex Alloys for Structural Nuclear Materials

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**ABSTRACT:**

Compositionally Complex Alloys (CCAs) represent a new region of composition space for metals and consist of four or more elements in single-phase solid solution, with no single element having a concentration less than 5 at% or higher than 35 at%. These new alloys have exceptional mechanical properties but for applications in nuclear technologies we need to dramatically increase our understanding of their irradiation response and corrosion behavior. The objective of this work is to develop understanding and predictive models for irradiation response and corrosion properties of selected structural Compositionally Complex Alloys (CCAs) relevant for high-temperature nuclear applications. We will realize this objective through three integrated thrusts focused on high-throughput (HT) synthesis and irradiation/corrosion (Thrust 1), HT and detailed characterization (Thrust 2), and atomistic and mesoscale simulation and machine learning (ML) (Thrust 3).

We will study FeCrMnNi, FeCrMoNi, MoNbTiV and MoNbTaW systems, which represent critical alloy spaces for cladding and structural applications, including models for traditional stainless steels (FeCrMnNi), Hastelloy (FeCrMoNi), and refractory alloys (MoNbTiV, MoNbTaW) for future high-temperature reactor concepts. Our HT synthesis will utilize in-situ alloying with directed energy deposition additive manufacturing (on a LENS MR-7). Irradiation effects in these materials will be studied with HT ion-irradiations making use of an innovative automated temperature-controlled stage with 2D motion at the UW Ion Beam Laboratory (IBL). HT oxidation vs. time and temperature for many samples will be made by exposing partially masked plates to high-temperature air conditions in the Co-PI corrosion laboratory. Characterization of irradiated and corroded will include very rapid HT characterization methods of nanoindentation (for hardening), profilometry (for swelling), plasma Focused Ion Beam (FIB) trenches for Electron Backscatter Diffraction(EBSD)/Energy Dispersion Spectroscopy(EDS)/3D-slicing (for oxide characterization of corroded specimen) and X-ray Diffraction (XRD) (for phase changes). Addition lower-throughput characterization will also be used to validate and interpret the HT method results, including accelerated characterization methods based on automated electron microscopy (for grain size, defect structure, and composition information), as well as selected detailed characterization with atom probe and transmission electron microscopy. These methods will provide an unprecedented database of irradiation and corrosion behavior on hundreds of samples in promising systems, enabling new access to trends with composition and irradiation/corrosion conditions. This database will be fit to machine learning (ML) models of key properties (e.g. hardness) vs. relevant features. Features in the ML models will include irradiation conditions (flux, fluence, ion type, energy, temperature, dpa profile), elemental composition, processing (e.g. annealing times), ab initio calculated properties related to irradiation/corrosion response (e.g., defect energies, stability of oxides), and results of approximate cluster dynamics models fit to the available data. The ML will be used to (i) identify novel features that can be determined easily, give new understanding of dominant factors, and provide a foundation for effective ML modeling, (ii) predict radiation/corrosion response for our alloy systems for situations not in our database to develop better performing alloys with less radiation/corrosion response, as well as attempt to predict trends in behavior of similar compositions to suggest promising alloys for future study (e.g., effects of adding Al). The HT experimental tools are already developed, and this proposal will focus on their application and the ML work. Almost all irradiation and characterization resources used are NSUF facilities.

The proposed work will produce (i) an unprecedented database of irradiation and corrosion behavior of CCAs, (ii) new understanding and predictive models for CCA irradiation and corrosion behavior, and (iii) a foundational example of the CHT methodology in structural nuclear materials. The proposed work will help the development of CCAs for structural nuclear applications and support the growth of CHT methodologies in nuclear materials research. The proposed research brings together 4 PIs who have the necessary skills, experience, and facilities to achieve the goals of this project: Morgan in molecular and mesoscale simulations and machine learning, Couet in advanced and high-throughput study of irradiated materials behavior and corrosion, Thoma in alloy design, high-throughput synthesis and advanced manufacturing, and Mukesh in advanced characterization and high-throughput sample preparation and characterization methods. The team has access to all necessary state of the art facilities through local and requested NSUF access, and are leaders, active users and developers at all the facilities proposed for use.