# Uncertainty Quantification and Management for Multiscale Nuclear Materials Modeling

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## ABSTRACT

Understanding and improving microstructural mechanical stability in metals and alloys is central to the development of high strength and high ductility materials for cladding and cores structures in advanced fast reactors. Design and enhancement of radiation-induced damage tolerant alloys are facilitated by better understanding the connection of various unit processes to collective responses in a multiscale model chain. The proposed work will address the question of propagating uncertainty associated with model prediction of material behavior under irradiation.

This project will consider quantification and propagation of both aleatory (irreducible) and epistemic (reducible) sources of uncertainty inherent in first principles, atomistics, and higher scale Monte Carlo and continuum crystal plasticity models of nuclear fuel and structural materials, with emphasis on mechanical properties/responses of irradiated ferritic alloys. Epistemic uncertainty associated with model assumptions, model structure, and estimates of the character/probability distribution of input parameters and model parameters will be made, facilitating sensitivity analyses. Special emphasis will be placed on quantifying uncertainty in nanostructures and microstructures under irradiation and the two types of uncertainties associated with structure-property predictions. The primary platform is a multiscale modeling framework that includes first principles and atomistic simulations of knock-on events with regard to remnant vacancy and interstitial fields and loop defects, the influence of interstitials on dislocation core spreading and mobility, Metropolis Monte Carlo and kinetic Monte Carlo (kMC) studies of collective unit processes to accumulate damage over higher length and time scales at elevated temperatures that are relevant to structures in service in the cladding and core assembly of advanced reactors, and a continuum crystal plasticity model that couples point defect and dislocation production/annihilation/migration, considering interaction with interstitial loops.

The project will incorporate uncertainty and error assessments within the length and time scales appropriate to each model to assess how this propagates through a chain of multiscale models. The primary theoretical vehicle to quantify the propagation of uncertainty is a generalized hidden Markov modeling approach based on a generalized interval probability theory. This method propagates solution sensitivities upward and downward in scale/level, and maps connections between various models in both directions, facilitating prioritization of further constitutive model refinement and the most critical subscale phenomena to model for several different model problems involving targeted objectives. The interplay of uncertainty propagation and the nature and degree of coupling between models at different scales (e.g., handshaking versus schemes for more direct transfer of information) will be explored. This will enable estimation of appropriate confidence bounds on performance predictions.