Project Title: Novel Nanostructured Coating Designs for Advanced Fuel Claddings Expedited by Modeling-Guided Approaches

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ABSTRACT:

Fuel cladding is a critical part of the fuel systems for the safe operation of nuclear reactors. Fuel cladding chemical interactions (FCCI) and cladding-coolant interactions could severely affect the cladding integrity and lead to premature failure of the fuel components. It is very challenging to have a cladding base material to meet all the requirements including neutron transparency, good thermal conductivity, high radiation tolerance properties, mechanical integrity and thermal and chemical inertness to fuels and/or coolants. Despite these preliminary successes in fuel cladding coating demonstrations by PI Wang and co-PI Gan, the knowledge gaps and design opportunities reside in the nitride coating exploration: (1) most of the nitride coatings on metallic claddings are nanocrystalline by nature by pulsed laser deposition (PLD) and sputtering under room temperature. Such nanocrystalline structures could offer significantly improved performance which are largely under explored. (2) specific atomic-scale interfacial characteristics at the nitride/metal interface are not yet clear which hinders the effective prediction and modeling effort. (3) the effects of nitrogen stoichiometry on the overall mechanical, oxidation resistance and corrosion resistance properties are yet to be explored. (4) the multilayer designs with interfaces as defect sinks for radiation-induced damage mitigation could be adopted in cladding coatings but need modeling and experimental validation.

Objectives: The PIs propose to combine experimental and modeling approaches to effectively explore the large design spaces offered by these naturally nanostructured nitride cladding coatings on metals, and take advantages of these nanostructure features to design superior cladding coatings for advanced nuclear reactors. The objectives of the project include: (1) to explore single phase nitrides and oxynitrides with tailored nitrogen stoichiometry in cladding coatings and its impact on the overall radiation tolerance, diffusion barrier properties, oxidation resistance, interfacial bonding, and mechanical integrity upon thermal cycling; This will be supported by atomic scale interfacial defect analysis by high resolution TEM/STEM coupled with EDX composition analysis to clearly reveal the defect nature at the nitride/metal interfaces. The important interface structures will inform the molecular dynamic (MD) simulations; Density function theory (DFT)-based interatomic potentials will be used for the MD simulations of the nitride/metal interfaces. Machine learning (ML) tools will be incorporated to develop new interatomic potentials from existing literature for composites and complex stoichiometry ones. (2) to establish interface structures using MD simulations for optimum multilayer designs and thus to apply modeling-guided multilayer designs to effectively engineer layer interfaces; Atomistic simulations based on the nudged elastic band method will be used to investigate the diffusion of defects to interfaces study and understand their impact on mechanical, radiation tolerance and damage properties, as well as diffusion barrier properties; (3) to design the nanocomposite coatings with multifunctionality using combinatorial experimental approaches, i.e., combi-sputtering and combi-pulsed laser deposition (PLD). Our ***overarching goal*** of the project is to accelerate the discovery of advanced nanostructured nitride-based coatings that address the diverse functionality needs in advanced nuclear reactors and establish a modeling framework for effective nitride/metal structures simulation and property prediction that can be applied to design effective coatings for other structural components in advanced nuclear reactors.