

## U.S. Department of Energy

## Functionally-graded Cermet and Metallic Coatings for Molten Salt Technologies by High Throughput Finite Element Modeling and Additive Manufacturing

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**ABSTRACT:** We propose an integrated approach/methodology to design, manufacture and verify functionally-graded ceramic-metal (cermet) and metal-metal composite coatings on structural alloys with desired interfacial properties, capabilities of mitigating residual stress and improved corrosion resistance for molten salt reactor (MSR) applications. The high temperature corrosion of molten fluoride salts presents a unique challenge for the application of structural materials. Strategies are developed to deposit metallic or ceramic coatings to improve corrosion resistance of Ni-based alloys in hot molten salts; however, the un-optimized coating design with mismatched properties and residual stress across the metal-metal or metal-ceramic interfaces may significantly degrade coating and materials performance. Functionally-grade coatings offer the opportunity to tune the properties across dissimilar interfaces to effectively mitigate residual stress and drastically improve materials performance. However, it becomes more expensive and technically impractical to search and test experimentally different combinations over a large design window with multiple structural parameters (e.g., coating thickness, composition/phase fraction, and architecture either in bilayer, multilayered discontinuous or continuous functionally graded coatings).

This project targets an integrated approach/methodology guided by high throughput finite element modeling (FEM) in coating design, which will be validated by combinatorial materials approaches and demonstrated by additive manufacturing (AM) to optimize and manufacture functionally-graded cermet and multilayered metal coatings. The key attributes of the optimized coatings include improved interface properties, reduced residual stress across dissimilar interfaces and exceptional corrosion resistance in hot fluoride salts. We will particularly focus on the design of the functionally-graded coatings on Hastelloy-N, the leading candidate for MSR technologies, and stainless steel (SS) 316. Multilayered functionally-graded cermet and metal coatings (e.g., metal nitrides or W) will be targeted with tunable CTEs with the alloy matrix and thus reduced residual stress from metal to metal and metal-to-ceramic coatings to achieve transformative performance. The high performance functionally-graded coatings will be demonstrated by two complementary AM approaches using laser cladding and thermal/plasma spray coating to validate and verification loop.

The optimization and verification of the high performance functionally-graded coatings on Ni super alloys or SS with transformative performance can greatly benefit to the safety and robustness of MSR operation and potentially significantly enhance the economics as more cost-effective SS may be applied for MSR applications. The high throughput FEM-guided coating design and optimization out of a broad design space coupled with high throughput materials synthesis and characterization and additive manufacturing can greatly accelerate materials discovery, testing and performance evaluation/verification. The developed methodology for coating design, demonstration and verification combining with high throughput continuum modeling, combinatorial materials approaches and additive manufacturing can be applied for a wide range of materials/coatings design for engineering applications beyond MSR technologies. Therefore, the proposed research is closely aligned with the mission of the AMMT program in strengthening new materials that can make advanced reactors more resilient and economically competitive. The collaboration with leading industries on additive manufacturing will greatly benefit to the development and implementation of new technologies for potentially engineering applications.