Simulation of Radiation and Thermal Effects in Advanced Cladding Materials

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ABSTRACT: The proposed work, supported by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program at Pacific Northwest National Laboratory, aims to implement a multiscale modeling scheme to improve our understanding of the phase stability and thermo-mechanical properties of nuclear fuel cladding under the combined effects of radiation, stress, and elevated temperature. The cladding material of interest is Fe-Cr-Al alloy. The goal is to connect atomic-level computer simulations and mesoscale methods to develop predictive physics-based models of thermal conductivity, swelling, and creep fin cladding materials. This proposal seeks a High Performance Computing allocation on the Falcon supercomputer to support NEAMS-funded work. This effort is supportive of an ongoing NEAMS High Impact Problem on accident-tolerant fuel led by Idaho National Laboratory and is also relevant to ongoing irradiation experiments in the Advanced Test Reactor.

We will use parallel molecular dynamics (MD) simulations enabled by a High Performance Computing allocation to study defect production and the initial stages in the formation of Cr-rich precipitates in Fe-Cr alloys, Monte Carlo simulations to study the nucleation of small Cr-rich clusters, and the phase field model to understand the growth and coarsening of these clusters. We will link these methods by transferring information between scales, such as interfacial energy, Cr diffusion coefficient, and cluster distribution. The proposed work will develop new understanding of precipitation and degradation of mechanical properties in cladding materials, complement ongoing experimental studies of cladding, and result in journal publications. Results from this work will be invaluable to the development of a much-needed ternary potential for eventually modeling Fe-Cr-Al alloys.

This work is well aligned with the mission of the NEAMS program to develop and deploy advanced computational tools for nuclear research and development. The proposed advanced computation involves a science based approach to Multiphysics modeling using high performance computing to better understand processes in nuclear materials. This effort addresses a current challenge of the Fuel Cycle Research and Development program, namely the development of improved cladding materials that can withstand prolonged irradiation and exhibit accident tolerance.