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Advancing the Underlying Science of Radiation-Tolerant Refractory Materials for Nuclear Energy Systems

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ABSTRACT

A collaborative investigation will probe the dynamics of the onset of radiation damage by coupling engineered nanomaterials, advanced microfabrication techniques, in situ electrical and optical measurement of radiation damage, and first-principles simulations. This unique collection of technical capabilities will create new in-situ methods to measure radiation damage accumulation and validate predictive models with particular attention to early stages of damage, investigate structure-property-radiation dosage relationships in material classes of scientific interest to advanced reactor applications, and mentor a cohort of new graduate and undergraduate students enthusiastic about the nuclear sciences.

The principal investigators (PIs) will present this information in a context that is relevant to the identification, engineering, synthesis, and performance prediction of next-generation refractory materials for advanced reactor applications. The material families of interest include refractory carbides, nitrides, and oxides. The content and structure of this proposed program are designed to meet both the programmatic needs of Department of Energy-Office of Nuclear Energy (DOE-NE) research efforts and the four programmatic goals of the Nuclear Energy University Programs (NEUP). This proposal will establish a new research link between three departments in two world-class U.S. universities and utilizes an existing user agreement between the research team and a DOE user facility that harnesses the powerful tools uniquely available to the U.S. national laboratory network.

The laboratory experiments and simulations will fabricate, irradiate, measure, and model basic electrical devices that integrate advanced reactor materials as active device components, thereby utilizing the incredible sensitivity of microelectronic devices to characterize radiation-induced material modifications at extraordinarily low doses. Two embodiments will be investigated: buried junctions and capacitors. In so doing, we leverage the synthesis tools of microelectronic fabrication and the investigative power of in-situ electrical and optical property measurements to provide transformative insight into radiation-solid interactions. The micron-scale thin-layer geometry provides an embodiment physically suitable for homogeneous irradiation while in-situ electrical testing provides the sensitivity to detect defects at concentrations several orders of magnitude below that visible to physical characterization tools like transmission electron microscopy. The integrated modeling effort will ensure that experimental findings are translated into fundamental process-property-performance relationships.

These methods offer a dramatic enhancement to the study of radiation-solid interactions beyond the conventional limitations of iterative irradiation and ex situ analysis. In situ property measurement will for the first time enable quantitative measurement of critically important parameters like defect accumulation rate, defect annihilation rate, and defect mobility at extremely low doses and as a function of temperature. This will create possibilities to explore metastable equilibria and identify phases stable only in extreme environments. Furthermore, we perceive promising opportunities to validate models that operate typically at short time scales,

specifically molecular dynamics (MD) and accelerated molecular dynamic (AMD) simulations. We believe that insight regarding these issues is tantamount to enhancing our understanding of radiation damage and our predictive abilities in this field.

The proposed research spans microelectronic devices, novel material synthesis, and advanced modeling and simulation and studies the overarching challenge of radiation tolerant materials for next generation reactors. This vibrant state-of-the-art program will create opportunities for students in these diverse fields to link their skills to a key nuclear engineering challenge, and thereby increase the pool of talented scientists and engineers that enter the nuclear industry. Finally, the makeup of this team includes two junior Nuclear Engineering faculty members and an associate professor of Material Science and Engineering who is currently entering his seventh year as a faculty member at the LUI. As such, this program will immerse three early career researchers in the nuclear sciences and actively address the need to mentor a new and sustainable generation of Nuclear Engineering educators and researchers.