NEUP | Nuclear Energy University Programs

U.S. Department of Energy

Radiation tolerance and mechanical properties of nanostructured amorphous-ceramic/metal composites

PI: Michael Nastasi
University of Nebraska-Lincoln

Program: Reactor Materials (NEET-3)

Collaborators: Michael Demkowicz, Massachusetts Institute of Technology; Lin Shao, Texas A&M University; Don A Lucca, Oklahoma State University

ABSTRACT:

The goal of this project is to use a radically non-traditional approach to design amorphous-ceramic/crystalline-metal composites for service in extreme irradiation environments. Rather than try to prevent microstructure changes in polycrystalline aggregates, the research team will evolve composite systems where one of the constituents is intentionally synthesized in a non-crystalline or "amorphous" state. Because amorphous materials possess no translational symmetry, such alloys do not contain conventional crystal defects such as vacancies, interstitials, or dislocations. These materials offer the possibility of eliminating the root cause responsible for radiation damage in polycrystalline solids - namely the production of point defects and clusters thereof in collision cascades - and may serve as the basis for developing a new class of structural materials with unprecedented resistance to radiation. The proposed amorphous/crystalline composites expect to achieve greatly improved radiation tolerance above 300 dpa (displacements per atom), stability above 500 ^{o}C, and improved mechanical performance combining the good properties of amorphous materials (high strength and elastic limit) with those of crystalline materials (high toughness, strain hardening). Another important feature of the proposed composites is the interface between the amorphous ceramic and metal, which—based on previous studies—is expected to be highly stable under irradiation. It is hypothesized that interfaces in these composite systems will be strong sinks for defects in the metal component, similar to what has been observed in metallic nanolayer composites, and for free volume in the amorphous component.

The ceramic component of the composite consists of a high crystallization temperature and radiation tolerant amorphous alloy composed of Si-C-O, while the metal layer will be Fe and Fe(Cr), chosen to serve as model materials for ferritic-martensitic steels. Previous work has shown that SiOC materials synthesized by this research team possesses both thermal and irradiation stability over a wide composition range, irradiation doses and irradiation temperatures. The material showed no evidence of crystallization up to a temperature of 1200 ^{o}C and an annealing time of 2.0 hours. Samples irradiated at both room temperature and 600 ^{o}C, highest temperature tested so far, showed no indication of crystallization or void formation .

In phase two of this work we propose the following research topics:

- Understand the role of Fe/SiOC interfaces on defect mitigation out to harsher environments with >300 dpa and >500 ^{o}C.
- Evaluate the role of SiOC and Fe(Cr)/SiOC interfaces on He incorporation.
- Further optimize compositions of SiOC ceramics and layered structures of Fe(Cr)/SiOC to achieve the maximum radiation tolerance, and determine the roles of Fe(Cr) and SiOC volume fractions on overall radiation tolerance and swelling resistance.

- In situ characterization of He retention using resonant Rutherford backscattering analysis and post irradiation characterization using atomic scale characterization (focused ion beam + transmission electron microscopy) to characterize interface configurations, defect clustering and void swelling, in order to link specific microstructures to corresponding radiation responses.
- Determine mechanical properties (hardness, elastic modulus and fracture toughness) of SiOC and SiOC/Fe(Cr) composites of various compositions, layer thicknesses, and volume fractions as a function of irradiation damage levels and irradiation temperatures.
- Multiscale modeling through integration of ab initio calculations and molecular dynamics simulations to shed light onto the interactions of defects and gas atoms with interfaces, and overall mechanical properties of composites. The study will identify the governing factors which determine the maximum radiation tolerance of the composite materials.
- Study the stabilities of boundaries under extreme radiation environment comparable to nuclear reactors, identify limits, and provide solutions to overcome the limits, in nanoscale design of radiation tolerant metal/ceramic composites.

The project fits into the NEET program for seeking crosscutting technologies which enables the development of new and advanced reactor designs and fuel cycle technologies. Advanced cladding or other suitable structural materials is urgently needed considering past accidents at Fukushima. Ceramic composites are therefore a strong option with steam reaction rates orders of magnitude lower than the Zircaloys currently in use. The project will provide an important contribution to the state of knowledge in reactor materials science, and enable significantly improved safety, performance and reliability for future advanced reactor designs. The project will lead to super-tough and ultra-high temperature resistant materials that are in critical need for nuclear applications under extreme conditions where in-core materials have to withstand neutron damage and high temperature. The project is built on a strong integration among four research groups from University of Nebraska-Lincoln for materials synthesis and characterization, Texas A&M University for high dpa irradiation testing and characterization, Oklahoma State University for mechanical properties evaluation and Massachusetts Institute of Technology for atomic scale modeling.