Study of Interfacial Interactions Using Thing Film Surface Modification: Radiation and Oxidation Effects in Materials

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ABSTRACT

Interfaces play a key role in dictating the long-term stability of materials under the influence of radiation and high temperatures. For example, grain boundaries affect corrosion by way of providing kinetically favorable paths for elemental diffusion, but they can also act as sinks for defects and helium generated during irradiation. Likewise, the retention of high-temperature strength in nanostructured, oxide-dispersion strengthened steels depends strongly on the stoichiometric and physical stability of the (Y, Ti)-oxide particles/matrix interface under radiation and high temperatures. An understanding of these interfacial effects at a fundamental level is important for the development of materials for extreme environments of nuclear reactors.

The goal of this project is to develop an understanding stability of interfaces by depositing thin films of materials on substrates followed by ion irradiation of the film-substrate system at elevated temperatures followed by post-irradiation oxidation treatments. Specifically, the research will be performed by depositing thin films of yttrium and titanium (~500 nm) on Fe-12%Cr binary alloy substrate. Y and Ti have been selected as thin-film materials because they form highly stable protective oxides layers. The Fe-12%Cr binary alloy has been selected because it is representative of ferritic steels that are widely used in nuclear systems. The absence of other alloying elements in this binary alloy would allow for a clearer examination of structures and compositions that evolve during high-temperature irradiations and oxidation treatments. The research is divided into four specific tasks: (1) sputter deposition of 500 nm thick films of Y and Ti on Fe-12%Cr alloy substrates, (2) ion irradiation of the film-substrate system with 2MeV protons to a dose of 2 dpa at temperatures of 300°C, 500°C, and 700°C, (3) oxidation of as-deposited and ion-irradiated samples in a controlled oxygen environment at 500°C and 700°C, (4) multi-scale computational modeling involving first-principle molecular dynamics (FPMD) and coarse-grained dissipative particle dynamics (DPD) approaches to develop theories underlying the evolution and stability of structures and phases.

Samples from Tasks 1 to 3 (above) will be rigorously characterized and analyzed using scanning electron microscopy, Auger electron microscopy, x-ray diffraction, Rutherford back scatter spectroscopy, and transmission electron microscopy. Expected outcomes of the experimental work include a quantitative understanding film-substrate interface mixing, evolution of defects and other phases at the interface, interaction of interfaces with defects, and the ability of the Y and Ti films to mitigate irradiation-assisted oxidation.

The aforementioned experimental work will be closely coupled with multi-scale molecular dynamics (MD) modeling to understand the reactions at the surface, the transport of oxidant through the thin film, and the stabilities of the deposited thin films under radiation and oxidation.

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Simulations of materials property changes under conditions of radiation and oxidation require multiple size domains and a different simulation scheme for each of these domains. This will be achieved by coupling the FPMD and coarse-grained kinetic Monte Carlo (KMC). This will enable the comparison of the results of each simulation approach with the experimental results.