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Neutron Radiation Effect on Diffusion between Zr (and Zircaloy) and Cr for Accurate Lifetime Prediction of ATF

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Abstract

One of the very promising accident-tolerant fuel (ATF) claddings for light-water reactors (LWRs) consists of Zircaloy coated with chromium (Cr). The diffusion coefficients – both impurity (dilute) diffusion coefficients and interdiffusion coefficients – between Zr (and Zircaloy) and Cr are essential for understanding and modeling the behavior of ATFs under operating and accident conditions as well as for accurate ATF lifetime prediction. A diffusion barrier interlayer of Mo, Nb, or Ta is also being explored to reduce the diffusion/reaction between Cr and Zircaloy under accident conditions. The objectives of this proposed project are: (1) to perform a systematic diffusion study of the Zr–(Cr, Nb, Ta, Mo) (and Zircaloy–Cr) as well as the Cr–(Nb, Ta, Mo) binary systems across the entire composition range at 6 temperatures ranging from 300 °C to 1200 °C to establish an unprecedented diffusion database for the 8 binary systems to fill a knowledge gap that currently exists due to insufficient data; (2) to perform neutron irradiation experiments at the temperature and neutron flux conditions close to the ATF operating conditions for extended durations at TREAT using the CINDI capsules such that the neutron-irradiated diffusion coefficients can be carefully evaluated; (3) to subtract the regular diffusion contributions from the neutron-irradiated diffusion coefficients so that the pure neutron irradiation effect on diffusion can be accurately evaluated for the 8 systems at 3 temperatures; and (4) establish an ATF diffusion coefficient database and to create a python code incorporating the resultant diffusion coefficients to allow engineers and researchers to simulate diffusion between Zircaloy and Cr with capabilities of including various thickness of interlayer (Mo, Nb or Ta) under various operating and accident conditions without or with neutron irradiation. Both the systematic dataset and the python code can be used to simulate various accident scenarios and operating conditions, optimize the ATF design (interlayer selection and thickness as well as Cr coating thickness), and thus help increase the robustness of Cr-coated ATFs against accidents.

The high-throughput diffusion-multiple approach and an enabling forward-simulation analysis (FSA) for diffusion coefficient extraction, both developed by the PI, will be leveraged to efficiently obtain the much-needed dataset. The proposed study will also demonstrate a novel efficient methodology of obtaining low diffusion coefficients by using atom probe tomography (APT) for steep gradient compositions and electron probe microanalysis (EPMA) for shallow gradient compositions. This integrated methodology will enable reliable extraction of diffusion coefficients (much) lower than 10^{-18} m^2/s without relying on the laborious tracer experiments, thus it will impact future diffusion research in nuclear science and engineering and beyond.

The project objectives will be achieved by executing 3 Tasks: Task 1—Make and analyze diffusion multiples, Task 2—Perform neutron irradiation experiments at 3 temperatures at TREAT as well as EPMA and APT at INL and Boise State University, and Task 3—Extract diffusion coefficients to build a diffusion database and create a python code for ATF diffusion simulation and lifetime prediction. PI and Project Director Zhao from The Ohio State University brings two decades of experience in diffusion studies and Co-PI Wu from Boise State University also brings two decades of experience in APT and several years of experience in working with neutron irradiated materials. The PIs will work closely with our Industry Advisor, Dr. Edward Lahoda from Westinghouse, to make the resultant data and the python code most relevant and impactful to ATF development in industry.