Characterization and Modeling of Grain Boundary Chemistry Evolution in Ferritic Steels

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ABSTRACT

Ferritic/martensitic (FM) steels such as HT-9, T-91 and NF12 with chromium concentrations in the range of 9-12 at.% Cr and high Cr ferritic steels (oxide dispersion strengthened steels with 12-18% Cr) are receiving increasing attention for advanced nuclear applications, e.g. cladding and duct materials for sodium fast reactors, pressure vessels in Generation IV reactors and first wall structures in fusion reactors, thanks to their advantages over austenitic alloys. Predicting the behavior of these alloys under radiation is an essential step towards the use of these alloys. Several radiation-induced phenomena need to be taken into account. In particular, radiation-induced segregation or depletion (RIS) at grain boundaries has raised significant interest because of its role in irradiation assisted stress corrosion cracking (IASCC) and corrosion of structural materials. Numerous observations of RIS have been reported on austenitic stainless steels where it is generally found that Cr depletes at grain boundaries, consistently with Cr atoms being oversized in the fcc Fe matrix. While FM and ferritic steels are also subject to RIS at grain boundaries, unlike austenitic steels, the behavior of Cr is less clear with significant scatter and no clear dependency on irradiation condition or alloy type. In addition to the lack of conclusive experimental evidence regarding RIS in F-M alloys, there have been relatively few efforts at modeling RIS behavior in these alloys. The need for predictability of materials behavior and mitigation routes for IASCC requires elucidating the origin of the variable Cr behavior.

A systematic detailed high-resolution structural and chemical characterization approach will be applied to both heavy ion implanted and neutron irradiated model Fe-5-14%Cr alloys containing controlled amounts of carbon (from <50ppm to 0.15wt.%). The combination of detailed experimental observations and atomistic modeling of Cr diffusion and point defect/solute interactions will be used understand the influence of grain boundary character and the presence of C on RIS of Cr, the role of Cr diffusion on grain boundary chemistry and its dependence on Cr concentration. The comparison of RIS in both types of implanted materials will indicate whether the trends observed in heavy ion irradiation hold for neutron irradiation and whether the theoretical models for Cr RIS in ion and neutron irradiation laboratory based studies can be extrapolated to advanced reactor operating conditions.

The objectives of the proposed work are therefore 1) to provide a fundamental and systematic experimental database of RIS in ferritic steels, by clarifying the relative effects of materials microstructure and irradiation conditions, 2) to develop a mechanistic understanding of the diffusion processes and solute/carbon interactions taking place explaining the behavior of Cr at grain boundaries, and 3) to benchmark atomistic models as predictive tools for the behavior of more complex alloy systems.

The combination of the proposed systematic experimental approach with atomistic modeling of diffusion processes directly addresses the programmatic need for developing and benchmarking predictive models for material degradation taking into account atomistic kinetics parameters.