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Impact of moisture on corrosion of NiCr alloys in $MgCl_2$-NaCl Salt Systems

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ABSTRACT:

Molten salt reactor (MSR) systems have attracted worldwide interests owing to their inherent safety, a strong negative temperature coefficient of reactivity, thermal and compositional stability, low pressure operation, and low production of nuclear waste. These unique features enable MSRs to operate at high temperatures and up to high burnups, thereby allowing for high thermal and fuel utilization efficiency. In MSRs, molten salts (MSs) are used either as coolant or both coolant and fuel solvent. Regardless of the design, all MSRs share a common challenge - corrosion of structural materials exposed to MSs at high operating temperatures, which can degrade the mechanical integrity of salt-facing components and lead to salt contamination. Albeit the substantial progress that has been made in developing corrosion resistant alloys, e.g., by the Aircraft Reactor Experiment (ARE) and the Molten Salt Reactor Experiment (MSRE) and follow-on efforts, fundamental understanding of corrosion mechanisms and corrosion kinetics is still urgently needed for timely development of corrosion resistance structural alloys. Corrosion in molten salts is driven by the impurities such as moisture (i.e., H_2O), not the salts themselves. *While previous experiments have shown moisture can significantly accelerate corrosion, it is unclear whether the impact comes simply from the amount of oxidizing species or from the changes in the corrosion mechanisms and kinetics.*

The objective of this project is to achieve a fundamental understanding of the effects of salt chemistry and moisture concentration on the mechanisms and kinetics of moisture-driven corrosion of NiCr alloys in molten $MgCl_2$-NaCl salts. By varying salt chemistry (i.e., $MgCl_2$:NaCl ratio) and H_2O concentration, the proposed research will: i) quantify salt chloro-acidity by coupling ab initio molecular dynamics (AIMD) simulations and ionic probe experiments using UV-vis spectroscopy, ii) determine the solvation structures of Cr ions and H_2O using AIMD, iii) determine the relative stability of Cr and its ions in salts using spectro-electrochemistry experiments, iv) compute the diffusivities of Cr ions and H_2O in the salts using AIMD, and v) investigate the initial stages of corrosion of Cr (i.e., the interaction between H_2O and Cr) at the salt/metal interface using AIMD. The outcome will bring in new knowledge on the role of moisture on corrosion of alloys in molten chloride salts of various compositions. Based on the new understanding, the correlation between H_2O concentration and corrosion kinetics will be established by coupling static corrosion experiments and multiphysics phase field simulations, to provide a critical piece of knowledge for assessing the integrity of structural alloys in molten salt reactors (MSRs). To ensure industrial relevancy, we will use salts provided directly by TerraPower and NiCr model alloys with different Cr contents representing Hastelloy N, Inconel 625, and Haynes 230, which are the primary candidates for MSRs and currently being considered for TerraPower's Molten Chloride Fast Reactor (MCFR). In addition, three PhD students will be trained at the collaborating universities, to develop highly trained scientists and support the future nuclear energy workforce. *Accomplishing the proposed research will advance the state-of-the-art modeling and experimental capabilities for studying molten salt corrosion mechanisms and kinetics and advance the current understanding, to support the development of structural materials in molten salt reactors.*