Optical Basicity Determination of Molten Fluoride Salts and its Influence on Structural Material Corrosion

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ABSTRACT:

Analogous to aqueous solution where the pH of solvent affects material corrosion in addition to redox potential, the basicity of molten salts also greatly influences the corrosion behavior of structural materials as well as other thermophysical properties, such as solubility, fission product speciation and stability, etc. The proposed research is aimed at developing ion probes to determine the optical basicity of molten fluoride salts and studying its influence on structural material corrosion. To quantify the basicity of molten fluoride salts, this proposed study will use transition metal ions, such as Tl^{+}, Pb^{2+}, and Bi^{3+}, as the probe ions. Through dissolving the selected probe cations in molten fluoride salts, the probe cations are coordinated by the fluorine atoms of molten fluoride salts and one can use that coordination to investigate the fundamental features of the salt chemical bonding. These fundamental features can be detected by Ultraviolet-visible spectroscopy (UV-Vis) signatures on the s-p spectra of the ion probe. To build the basicity scale, the LiF will be chosen as the unity optical basicity. Based on the frequency obtained on the s-p spectra for different fluoride salt mixtures after the addition of the ion probe, the optical basicity can be defined by a model as already well developed for molten glass system. By using the developed ion probes, different molten fluoride salts including eutectic, and off-eutectic, FLiNaK (LiF-NaF-KF) and FLiBe (LiF-BeF_2), with and without additions of lanthanide/actinide fluorides will be determined. To achieve the high throughput measurement on the basicity of molten fluoride salts with different chemical constituents, a special chemical titration will be designed for the addition of different amounts of chemicals such that the optical basicity of a variety of salt mixtures can be obtained in-situ by the equipped UV-Vis. With the accumulation of optical basicity data for a variety of molten fluoride salts, basicity moderating parameter will be calculated and the correlation between optical basicity and salt composition can be derived. To understand the physical and chemical features controlling the optical basicity variations with chemical compositions in a molten salt system, the structures of molten salts with different compositions will be investigated by Extended synchrotron X-Ray Absorption Fine Structure (EXAFS) and X-Ray Absorption Near-Edge Structure (XANES) in terms of bonded complexes, coordination number, interatomic distance, and mean-squared disorder. The influence of optical basicity on structural material corrosion will be studied through the isothermal corrosion experiment of commercial alloys in molten fluoride salts of interest with different optical basicity. For comparison, all the corrosion experiments will be performed at the same condition. A spectro-electrochemistry test cell will be designed for quantitative and speciation-specific measurement of dissolved corrosion products and achieving the in-situ corrosion monitoring during the corrosion experiment. The corroded samples after corrosion experiment will also be analyzed by post-corrosion characterization using a suite of materials analysis techniques.