Modeling Radiolysis Effects in FLiNaK and FLiBe Molten Fluoride Salt

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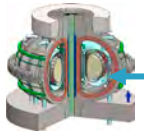
Introduction

Next generation fission and fusion reactors will use molten salts as key functions in their reactor design. To better understand the behavior of molten salt in a reactor environment, we investigate the fundamental mechanism(s) of how radiation affects corrosion in FLiNaK and FLiBe.

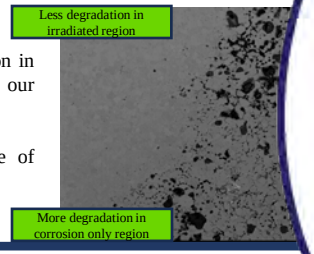
FLiNaK used as Fuel and/or Coolant

FLiBe as Fusion Breeding Blanket



Our group has discovered radiation *decelerated* corrosion in molten fluoride salts. To further understand this affect, our study aims to answer two main questions:

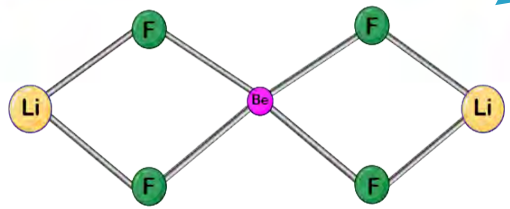
(1) How does radiation affect the chemical structure of FLiNaK and FLiBe?
(2) Will radiation affect the corrosion rates of these salts?



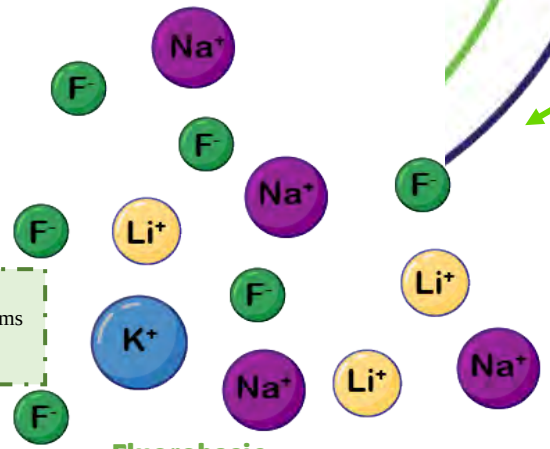
Research Highlights

Fluoroacidic

Pre-irradiation FLiBe is fluoroacidic (below)



FLiNaK is fluorobasic (below)

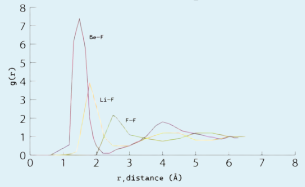


Fluorobasic

Hypothesis

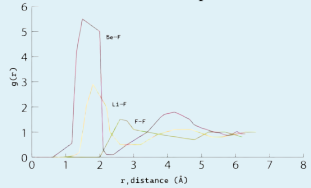
We expect that radiation will break down FLiBe's tetrahedral ionic clusters, causing fluorine dissociation and making the salt more fluorobasic. However, in FLiNaK, fluorine is already dissociated with no local structure. We expect irradiation effects to be small.

FLiBe structure – pre-irradiation



Irradiation

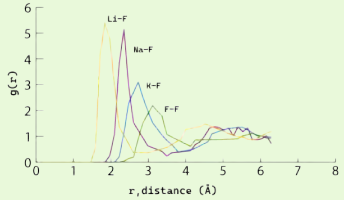
FLiBe structure – post-irradiation



Structure determined using Molecular Dynamics simulation

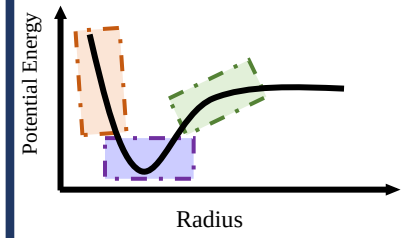
Example of expected structure (work in progress)

FLiNaK structure– pre-irradiation; no expected change post-irradiation



Methods

We use a machine learning based interatomic potential (ML-IP) to predict initial configurations, then simulate irradiation by imparting high kinetic energy to an atom.



Equilibrium
Provides structural and thermodynamic properties

Repulsive
non-equilibrium properties (atoms slamming into each other from irradiation)

Attractive
non-equilibrium properties (atoms pulled apart by irradiation, breaking local structure)

ML-IP was previously developed using Ab-Initio Molecular Dynamics, to sample the equilibrium and non-equilibrium regions (e.g., attractive and repulsive). We then used molecular dynamics to simulate irradiation and calculate molten salt properties.

Discussion and Conclusions

We expect to find that irradiated FLiBe will present a larger increase in relative corrosion compared to irradiated FLiNaK. This will improve our understanding of radiation-induced corrosion in molten salt, and further helps us design better materials for fission and fusion reactors.

The radial distribution function (RDF) for FLiNaK and FLiBe is expected to indicate an increase in fluorobasicity, based on the pF scale for FLiBe, and small increases in fluorbasicity for FLiNaK.

$pF = -\log(a_f)$
Fluoroacidity (pF) based on free fluorides content

Amongst other factors, it is suspected that FLiBe becoming more fluorobasic may correlate to an increase in relative corrosion rates. We anticipate this analysis will serve as a foundational assessment to understand the effects of radiolysis in both FLiNaK and FLiBe corrosion.