Materials Science & Engineering and Metallurgical Engineering Graduate Seminar

Wednesday, November 21, 2018, 4:10-5:00PM, WEB 1230

Nora Alnajjar, PhD candidate, METE

Electrodeposition of U and Th from Molten LiCl-KCl onto a Pt Surface for Actinide Monitoring Using Alpha Spectroscopy

In order to develop a sensor for measuring actinide concentrations in molten electrorefiner salt, a process for electrodeposition of U and Th from LiCl-KCl-UCl3-ThCl4 onto Pt-coated surfaces has been developed. To facilitate the counting of alpha particles by the sensor, the objective is to electrodeposit a uniform, one micron thick layer of actinides. Such a deposit was accomplished using repeating chronoamperometry (RCA) tests in LiCl-KCl-UCl3, LiCl-KCl-ThCl4, and LiCl-KCl-UCl3-ThCl4 molten salt mixtures at 500⊠C. Uniformity of the deposits was verified using scanning electron microscopy with energy dispersive x-ray spectroscopy (SEM-EDXS). Time to pass a fixed amount of electric charge through the cell was correlated with concentrations of UCl3 and ThCl4 in the salt mixtures. As expected, the deposition time was inversely proportional to actinide concentration in the salt. The actinides could be stripped and re-deposited multiple times on a given Pt-coated coupon with repeatable time results. This method shows great promise for simultaneously measuring concentrations of multiple actinides with very close electrochemical reduction potentials. It thus offers potential functionality beyond what is possible with only electrochemical methods such as cyclic or normal pulse voltammetry.

Nora Alnajjar is a graduate student in Dr.Simpson's Nuclear Pyrometallurgy Lab. She is working on her master's degree in metallurgical engineering. After graduation, she hopes to continue working with electrochemistry and molten salts in the nuclear industry.

Jake Graser, PhD candidate, MSE

Breadth vs Accuracy of Predicting Across Many Crystal Structures

Predicting crystal structure has always been a challenging task for physicists, chemists, and material scientists. From Pauling to Villars, we have made significant progress in outlining rules for the formation of crystal structures. However, we still lack the ability to predict crystal structure from formula alone. Therefore, modern techniques utilize energy-based computational approaches in calculating crystal structure and have proven successful. However, these have limitations when it comes to crystal structure predictions such as computational time and requiring a starting crystal structure. Recently, machine learning has shown notable success in predicting crystal structures. Yet, these algorithms have been limited in scope, only being able to predict within a realm of a specific crystal structure. In this presentation, I will give an overview of machine learning as well as our efforts to build a machine learning algorithm to predict across multiple crystal structures. I will outline how accuracy, precision, and recall are determined as well as discuss how increasing prediction breadth affects accuracy of the algorithm. Jake Graser is a PhD student at the University of Utah. He received his Bachelor's degree in Applied Physics from the University of Utah in 2011 and his Master's degree in Material Science from Arizona State University in 2013. His research interests are materials focused machine learning as well as thermoelectric devices.