Probing Multiscale Transport and Inhomogeneity in a Lithium-Ion Pouch Cell Using In-Situ Neutron Methods

**Achievement:** A powerful nondestructive tool that can be utilized to understand the multiscale nature of lithium transport is developed with combined in-situ radiography and diffraction supported by 3D multiscale electrochemical modeling.

**Significance and Impact:** This work improves our ability to effectively analyze in-homogeneities of a thick electrodes during various states of lithiation at a cell level that are important for increasing energy density of batteries.

**Research Details:**
- This study utilizes neutron imaging contrast to spatially observe lithium transport across thick graphite electrodes at various states of lithiation in a pouch cell configuration
- Neutron radiography/imaging profiles measure the change in the optical density (OD) or contrast and an attempt has been made for the first time to correlate the changes in OD upon lithiation to local lithium concentration profiles calculated using 3D electrochemical transport modeling.

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**Overview:**
We demonstrate the lithiation process in graphitic anodes using in-situ neutron radiography and diffraction in a single-layer pouch cell. The variation in neutron absorption contrast in graphite shows a direct correlation between the degree of lithiation and the discharge potential. The experimental neutron attenuation line profiles across the graphite electrode at various discharge times (potentials) were compared with lithium concentration profiles computed using a 3D electrochemical transport model. In conjunction with imaging/radiography, in-situ neutron diffraction was carried out to obtain information about the local structural changes during various stages of lithiation in carbon. Combined in-situ radiography and diffraction supported by 3D multiscale electrochemical modeling opens up a powerful nondestructive tool that can be utilized to understand the multiscale nature of lithium transport as well as observe various in-homogeneities at a cell level.