Contribution ID: **99** Type: **Talk**

Architectural Variations of Li2MnO3-Li0.69MnO2 Core-Shell Cathodes During the Cycling Process

Wednesday, 3 December 2025 13:50 (20 minutes)

The core-shell architecture has garnered significant interest for electrode materials owing to the ability to enhance conductivity, stability and enhanced surface functionality. Due to its high capacity and energy density, the O3-type Li2MnO3 layered cathode material is a potential candidate electrode for large-scale energy storage. However, it tends to undergo structural transformation from layered to spinel configuration during charge cycles due to irreversible oxygen loss. Recent advances in surface coating techniques have improved the electrochemical performance of these cathodes by enhancing conductivity, stabilizing structures, and preventing harmful reactions with the electrolyte. One of the setbacks with this strategy is the delamination of the core from the rigid shell attributed to the radial tensile radial stress on the interface of the core shell. This compromises the mechanical integrity of the core-shell structure and affects the electrochemical performance of LIBs. In this study, Li2MnO3 is coated with Li0.69MnO2 for the first time, a layered material known for its stability (no phase transformation) and high ionic conductivity. Molecular dynamics simulations, using the DL_POLY code, were employed to examine the cycling performance of the Li2MnO3-Li0.69MnO2 core-shell system by delithiated from Li2MnO3 to LiMnO3 and to closely monitoring the potential risk of delamination under various temperature conditions. The simulations were carried out using the Nose-Hoover thermostat under the NVT ensemble with temperatures ranging from 300 K to 1500 K. The structural snapshots obtained indicated a fluctuating pattern in the system's structural stability at different temperatures. Notably, at certain temperatures, the core-shell system lost a significant number of atoms from both the core and shell, while at other temperatures, the system regained order with minimal atom loss. Additionally, the lithium diffusion coefficients varied with lithium concentration, showing higher diffusion values for Li1.3MnO3 and Li1.7MnO3 at lower temperatures and Li1.4MnO3 demonstrated highest diffusion rates of 1.25 nm/s2 at 1500 K whilst the highest attainable diffusion was that of Li1.7MnO3, 3.02 nm/s2 at 1200 K. Overall, temperatures where greater atom loss occurred show high diffusion though this trend was not consistent across all concentrations. The simulations were conducted using 48 cores and 5 nodes.

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Session Classification: HPC Applications