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Analysing Core-Shell Compatibility During the Cycling Process Using Molecular Dynamics Simulations

The O3-type Li_2MnO_3 layered cathode material shows great potential for large-scale energy storage in electric grids and vehicles due to its high capacity and energy density. However, it tends to undergo structural changes from a layered to a spinel configuration during charge cycles. 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. However, the core-shell configuration in surface-coated materials still suffer mechanical degradation caused by interfacial stress. The radial tensile stress at the core-shell interface can lead to delamination of the coating layer, weakening the structural integrity of the cathode and negatively impacting the long-term performance of lithium-ion batteries. In this study, Li_2MnO_3 is coated with $\text{Li}_{0.69}\text{MnO}_2$, a layered material known for its phase stability and high ionic conductivity. Molecular dynamics simulations, performed using the DL_POLY code, were utilized to analyse the cycling performance of the Li_2MnO_3 - $\text{Li}_{0.69}\text{MnO}_2$ core-shell system and assess the potential risk of delamination under various temperature conditions. During the simulations, the core was delithiated from Li_2MnO_3 to LiMnO_3 . The Nose-Hoover thermostat under the NVT ensemble was used, with temperatures ranging from 300 K to 1500 K. Structural snapshots revealed fluctuations in system stability at different temperatures. At certain temperatures, the core-shell system experienced significant atomic loss from both the core and shell, whereas at other temperatures, it regained structural order with minimal atom loss. Lithium diffusion coefficients varied with lithium concentration, with $\text{Li}_{1.3}\text{MnO}_3$ and $\text{Li}_{1.7}\text{MnO}_3$ exhibiting higher diffusion at lower temperatures, while $\text{Li}_{1.4}\text{MnO}_3$ showed the highest diffusion rate of $1.25 \text{ m}^2/\text{s}$ at 1500 K. The maximum recorded diffusion occurred in $\text{Li}_{1.7}\text{MnO}_3$ at 1200 K, reaching $3.02 \text{ m}^2/\text{s}$. Overall, higher atom loss corresponded to increased diffusion, though this trend was not consistent across all concentrations. These results highlight the balance between lithium diffusion and structural integrity, offering key insights for improving the durability of coated cathode materials in advanced lithium-ion batteries.

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