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The Structural Variations of Li1+xNi0.5Mn1.5O4 Nanoporous Material for Li-ion Battery Cathodes

The demand for batteries with higher energy density and storage capacity has been increasing over the past three decades. As such, spinel LiMn2O4 has emerged as one of the most promising cathode materials for Li-ion batteries, owing to its environmental friendliness, inexpensiveness, and structural stability compared to its counterparts, such as LiCoO2. However, LiMn2O4 suffers from high capacity loss and voltage fade due to factors such as the Jahn-Teller distortion and disproportionation reactions, which cause volume expansion in bulk materials. This results in a material that has reduced symmetry and energy, consequently causing fractures and pulverisation to the material. Studies have shown that Ni doping can mitigate the specific capacity loss and voltage fade in LiMn2O4 cathodes and improve their structural stability. Furthermore, nanoporous materials as electrodes offer a large surface area and pore volume for better electrolyte interaction and Li+ diffusion, resulting in enhanced electrochemical performance and mechanical stability. Therefore, in this study, molecular dynamics (MD) simulations using the DL_POLY code are employed to investigate the structural changes on lithiated and Ni-doped Li1+xNi0.5Mn1.5O4 nanoporous material with 67x67x67 Å cell dimension. The nanoporous material has recrystallised into single and multi-grained structures during lithiation. The pore cavity of the material is reduced or completely closed with the Ni dopant and increasing Li content. Furthermore, the surface areas of the material increased with lithiation except at the abrupt concentration of Li1.75Ni0.5Mn1.5O4; in this Li concentration, the surface areas reduced significantly. In addition, the material expands with increasing Li concentration; however, the structural integrity of the material is maintained upon full lithiation. This is because the material almost regains its porosity and recrystallizes into single-grained structures. This indicates that Ni-doped LixMn2O4 nanoporous materials can potentially stabilise and retain the spinel structure to enhance their cycling stability.

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