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Investigating the Structural and Volume Changes of Composite Layered–Spinel Nanoporous Li-Mn-O Electrode Materials

Nanoporous material for lithium ion batteries cathodes have currently drawn much attention than the bulk due to their improved electrochemical performances and mechanical stability. Layered-spinel lithium manganese oxides (LMOs) have also become the most desirable cathodes owing to their spontaneously great reversible capacity (302 mAh/g) and superior rate capability. Herein, we present the host capability of the Li-Mn-O nanoporous composite material which was simulated to predict the behaviour of the layered-spinel composite cathode during the discharge process by employing the amorphization and recrystallization technique, using the computer code, DL_POLY.
The total RDFs and structural snapshots for the Li-Mn-O composites showed efficient spontaneous recrystallization at different concentrations of lithium. The microstructures and XRD patterns showed spinel and layered components co-existing in the nanostructure. Increment of the Li content resulted in polycrystalline structures (88% lithium concentration), reduction in defects and is favourable for the layered-spinel content. However when the structures are fully lithiated (100% lithium concentration), their polycrystalline nature is reduced or lost completely. The NST ensemble was employed and it was observed that the nanoporous materials expands within their pores as the lithium concentration is increased.

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