63rd ANNUAL CONFERENCE OF THE SA INSTITUTE OF PHYSICS

Contribution ID: **54** Type: **Oral Presentation**

Effects of pore size on the electrochemical properties of Li-Mn-O nanoporous cathode material

Tuesday, 26 June 2018 12:00 (20 minutes)

Nanoporous spinel materials have ignited interest as cathode materials for lithium ion batteries owing to their superior rate capability at ambient temperature, improved electrochemical performance and mechanical stability, compared to the bulk material. However, nanospherical layered-spinel lithium manganese oxides (LMOs) cathodes have demonstrated spontaneously great reversible capacity (302 mAh/g) and superior rate capability due to their composite nature. In this study we simulated the synthesis and investigate the host capability of various Li-Mn-O nanoporous composite materials. The prediction of electrochemical behaviour of these layered-spinel composite cathodes, during the discharge process of a lithium ion battery, is carried out by employing the amorphization and recrystallization technique, using the DL_POLY code. The radial distribution functions (RDFs), X-ray diffraction patterns (XRDs) and structural snapshots of various microstructures for the Li-Mn-O composites showed efficient spontaneous recrystallization (exothermic) and co-existence of spinel and layered components in the nanoporous materials with different pore sizes. Increment of the Li content resulted in more polycrystallization structures and increment of the layered content in the nanostructures.

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Session Classification: Physics of Condensed Matter and Materials

Track Classification: Track A - Physics of Condensed Matter and Materials