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The simulated synthesis of nanostructured Li2MnO3 cathode materials

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The realisation of advanced lithium-ion battery (LIB) technologies has been hindered by the slow progress in discovering high capacity cathodes. Considerable research is focused on the lithium-rich layered Li2MnO3 owing to its ability to reversibly intercalate more lithium. However, the cycling of this material results in capacity degradation due to complex phenomena such as the irreversible oxygen loss and phase transformation caused by lattice reconstruction. Herein, a series of nanostructured Li2MnO3 models have been generated via the simulated amorphisation and recrystallisation (A+R) technique and their internal microstructures interrogated during the cycling process. The charging process involved the concurrent removal of lithium (Li) and oxygen (O) ions to restrain the release of oxygen and resulted in Li2-xMnO3-x composites. Detailed analysis of these composites reveals that the models crystallised into multiple grains which increased with decreasing Li/O content along with stacking faults and vacancies thus leading to Mn ions migrating to the Li layers. The internal microstructures display a wealth of defects leading to the emergence of distorted cubic spinel LiMn2O4, Li2MnO3 and LiMnO2 polymorphs. Characterisation of the x-ray diffraction patterns revealed peak broadening along with the growing of 2Θ˜18-25 and 2Θ˜29⁰ peaks associated with the spinel-like phase. These results shed insights on the mechanism that takes place during the cycling of the Li2MnO3 with complex structures and will help guide the optimisation of high-capacity energy storages.

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Yes

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Primary authors: Mrs MOGASHOA, Tshidi (UL); LEDWABA, Raesibe Sylvia (University of Limpopo); NGOEPE, Phuti (University of Limpopo)

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