SIMULATED SYNTHESIS AND CHARACTERISATION OF Li-Mn-O NANOSTRUCTURES

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Simulated amorphisation recrystallization methods, are now routinely used to generate models of various nano-architectures for metal oxides with complex microstructural details [1,2]. In the current studies the approach is used to generate nanostructures of manganese dioxides, and those associated with the Li_2MnO_3 and spinel $LiMn_2O_4$ for Li-ion battery application. Firstly, lithium transport and mechanical properties of pure and lithiated nanorods and nanoporous MnO_2 are discussed and compared with the bulk structure. In particular, stresses related to lithium insertion and how these impact on electrochemical properties are outlined. Secondly, a nanosphere of the ternary Li_2MnO_3 was synthesised and molecular dynamics (MD) simulations of its charging reveal that the reason nanocrystalline-Li_2MnO_3 is electrochemically active, in contrast to the parent bulk-Li_2MnO_3, is because in the nanomaterial the tunnels, in which the Li ions reside, are held apart by Mn ions, which act as a pseudo ópoint defect scaffoldô. Lastly, nano-architectures, i.e. nano- sphere, sheet, porous and bulk, associated with the Li-Mn-O ternary were synthesised from amorphous spinel nanosphere. The resulting crystallised nanostructures are characterised from visual images, radial distribution functions, XRDs and simulated microstructures. A preliminary analysis reveals the presence of the layered Li_2MnO_3 and spinel $LiMn_2O_4$ together with a wide variety of defects, including grain boundaries and ion vacancies.

References:

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