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The effect of partial sodium substitution on the lithium site of the Li_2MnO_3 cathode materials for lithium-ion batteries

The layered Li_2MnO_3 has attracted tremendous research interest as a cathode material for high capacity lithium-ion batteries due to its high theoretical capacity of 459 mAh.g^{-1} and the ability to reversibly intercalate more lithium. However, voltage decaying and poor rate capability during cycling pose serious problems in its practical application. To solve this problem, sodium-ion substitution in the lithium site has been reported to be an effective approach to facilitate the conductive ion diffusion rate of Li-rich layered materials and thus to improve their rate capacity. In this work, the nanostructured Li_2MnO_3 models have been generated via the simulated amorphisation and recrystallisation (A+R) technique employing the DL_POLY code. Accordingly, sodium was partially introduced into the Li_2MnO_3 lattice resulting in a series of $\text{Li}_{2-x}\text{Na}_x\text{MnO}_3$ ($0 \leq x \leq 2$) models of different lithium and sodium content. Amorphisation and recrystallisation were carried out at temperatures between 1600-1800 K. Characterisation of the x-ray diffraction patterns revealed peak broadening along with the shifting of peaks to the right due to the enlarged lithium layers occupied by sodium ions to facilitate lithium diffusion. Consequently, lithium diffusion in sodium-substituted systems was found to be higher as compared to the pristine Li_2MnO_3 . These results shed insights on the role of sodium on the layered Li_2MnO_3 models.

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