

Poster Presentation

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Atomic structure of $\text{Li}_{2-x}\text{MnO}_3$ studied by neutron diffraction and STEM

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Li_2MnO_3 is an important cathode material with extra high capacity ($>300\text{mAh g}^{-1}$ for the first charge process). The exact charge-discharge mechanism and the structure evolution still remain controversial. Here the atomic structures of Li_2MnO_3 after partial delithiation and lithiation are investigated by neutron powder diffraction and spherical aberration-corrected scanning transmission electron microscopy (STEM). Neutron diffraction experiments are performed on $\text{Li}_{2-x}\text{MnO}_3$ ($x=0, 0.25$) in a bulk level. It can be found that the volume of the unit cell almost keeps constant, while the lattice constants in the a, b direction increases after the chemical delithiation, but the c direction decreases. For the delithiated compound $\text{Li}_{1.75}\text{MnO}_3$, the Li occupancies are $0.7(+0.3)$, $0.9(+0.1)$ for the 2c and 4h sites, respectively, resulting in the Li-concentration of $1.75(+0.27)$, while the 2b sites are fully occupied. Furthermore, the isotropic thermal vibration factors of the 2c and 4h Li atoms are considerably larger than that of the 2b Li atoms, also seemingly implying the feasible delithiation of Li atoms at the 2c and 4h sites in the Li-O layer. It is interesting to note that the thermal factor of Mn atoms is slightly larger than O atoms, which probably means that the Mn atoms are more mobile than O atoms. The STEM results suggest that the Li ions can be extracted both from the LiMn_2 planes and Li planes, and the Mn ions can move reversibly in the (110) plane during delithiation and lithiation.

Keywords: lithium battery material, neutron diffraction, STEM