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Atomic Resolution of Lithium Ions in $LiCoO_2$

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It is well known that ultra high-resolution is needed to resolve light elements in a heavy-atom matrix, such as Li^+ in a transition metal oxide. Recent advances in high-resolution transmission electron microscopes (TEM) and associated software, particularly exit-surface wave (ESW) reconstruction, push the resolution limit to better than 0.1nm, which provides opportunities to examine whether Li^+ could be imaged and resolved in a transition metal oxide structure. A layered $LiCoO_2$ compound with space group R-3m was studied here, prepared from a mixture of Li_2CO_3 and Co_3O_4 at 900°C in O_2 for 24hrs. It was found from exit-surface wave (ESW) simulations that a microscope resolution of 0.1nm was needed to experimentally resolve individual lithium ions in the layered structure along the [110-2] zone axis for specimen thickness close to 5nm. Application of neutral Li and charged Li^+ scattering factors in the calculations led to no considerable difference in the ESWs. The simulation results were then compared with focus-series reconstructed ESWs along the [110-2] zone axis. The ESWs were reconstructed from several focus-series of experimental TEM images using the Philips/Brite-Euram software, which were obtained on a modified Philips CM300FEG/UT microscope with a native resolution of 0.17nm and a demonstrated maximum resolution of 0.078nm. It was found consistent with the simulation results that the intensity associated with the Li^+ position in the experimental ESWs was the weakest in comparison to those of oxygen and cobalt. Simulations from a model with no Li^+ present showed no contrast at the Li^+ position. Therefore, both simulation and experimental results support the fact that Li^+ was resolved atomically in $LiCoO_2$.
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