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Publication Date

2003-01-24

Image Simulation and Experimental Resolution of Li⁺ in LiCoO₂

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Image Simulation and Experimental Resolution of Li⁺ in LiCoO₂

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Advances in high-resolution transmission electron microscopes (TEMs) and associated software, particularly exit-surface wave (ESW) reconstruction of the scattered electron wave, push the resolution limit to better than 0.1nm, which provides opportunities to examine whether Li⁺ can be imaged and resolved in a transition metal oxide structure. From simulations of the exit-surface wave (ESW) generated by structural models of LiCoO₂, it was found that a microscope resolution of 0.1nm was needed to experimentally resolve individual lithium ions in the layered structure. The phase of the ESW is a function of the specimen potential (projected atom density). Our simulations show that the ESW phases of the lithium, cobalt and oxygen atom columns change almost linearly with specimen thickness. The simulated ESWs were then compared with experimental ESWs reconstructed from experimental focus-series along the [110] zone axis. Reconstructions were carried out, using the Philips/Brite-Euram software, from several focus-series of 20 TEM images obtained on a modified Philips CM300FEG/UT microscope with a native resolution of 0.17nm and a demonstrated reconstructed ESW 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. Both simulation and experimental results support the fact that Li⁺ was resolved atomically in LiCoO₂.

ACKNOWLEDGMENTS

National Science Foundation International Research Fellow Award INT-0000429 is acknowledged. This work was partially supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division, U.S. Department of Energy under Contract No. DE AC-03-76SF00098.