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Author

Delmas, Claude

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Atomic Resolution of Lithium Ions in LiCoO₂

Y. Shao-Horn^a, M.A. O’Keefe^b, E.C. Nelson^b, L. Croguennec^a and C. Delmas^a

^a Institut de Chimie de la Matière Condensée de Bordeaux-CNRS and
Ecole Nationale Supérieure de Chimie et Physique de Bordeaux
Université Bordeaux I
33608 Pessac cedex, France

^b National Center for Electron Microscopy
Lawrence Berkeley National Laboratory
Berkeley, CA 94720, USA

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^a Institut de Chimie de la Matière Condensée de Bordeaux-CNRS and
Ecole Nationale Supérieure de Chimie et Physique de Bordeaux
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33608 Pessac cedex, France

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Berkeley, CA 94720, USA

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 LiCoO₂ compound with space group R-3m was studied here, prepared from a mixture of Li₂CO₃ and Co₃O₄ at 900°C in O₂ 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 LiCoO₂.