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Near-field Nanoscopy and Spectroscopy of Phase Coexistence in $LiFePO_4$ Electrode Microcrystals IVAN T. LUCAS, University Pierre and Marie Curie, Paris, France, ALEXANDER MCLEOD, University of California, San Diego, JAROSLAW S. SYZDEK, Lawrence Berkeley National Laboratory, DEREK S. MIDDLEMISS, University of Cambridge, ROBERT KOSTECKI, Lawrence Berkeley National Laboratory, D.N. BASOV, University of California, San Diego — Due to instrumental limitations, the microscopic description of lithiation and delithiation processes in low-cost $LiFePO_4$ electrodes has remained uncertain and subject to controversy. Using infrared near-field imaging, we present evidence for a novel coexistence of phases within single $LiFePO_4$ microcrystals. First-principles calculations of the phonon response of lithiated and delithiated end-phases are compared with broadband nano-FTIR (Fourier transform infrared) spectroscopy data to reveal the mid-infrared vibrational signature of lithiation. By resolving this signature at the nano-scale, we observe a propagation of phase boundaries within these crystals over the course of chemical delithiation. In addition, by comparing theoretical modeling with spatially resolved nano-FTIR spectra measured across a single crystal at partial delithiation, we assemble a tomographic view of phases distributed hundreds nanometers beneath the crystal surface. These experiments set the stage for quantitative nano-spectroscopy of new composite electrode materials, assisting in the rational design of next-generation electrical energy storage systems.

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