

Engineering electron density and structural properties of CuO anode material via calcination and in situ synchrotron XRD for enhanced lithium-ion battery performance

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Abstract

This research focused on engineering the electron density distribution and structural characteristics of CuO, including stacking fault probability, lattice strain, crystallite size, and dislocation density, through calcination to enhance the electrochemical performance of lithium-ion batteries (LIBs) when used as anode electrodes. The CuO material was synthesized by the simple and convenient chemically precipitated technique. Techniques such as laboratory X-ray diffraction (XRD), synchrotron X-ray diffraction (SXR), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS) confirmed the formation of CuO. The electron density distribution and structural properties were analyzed via XRD and SXR Rietveld refinement. The results indicated that the optimal electrochemical performance was achieved with CuO calcined at 400 °C. In situ SXR characterization of this CuO was performed to investigate its crystallographic parameters and stability over temperature range from – 100 to 600 °C. The crystal structure contracted and expanded for lower and higher temperatures, respectively, in comparison with room temperature. The CuO-400 anode exhibited better electrochemical performance, achieving a specific discharge capacity of 2751.7 mA h g⁻¹ at a rate of 1.0 C, approximately a 50% improvement over the as-synthesized CuO anode. After 100 cycles, CuO-400 electrode at 400 °C delivered a specific discharge capacity of 364.2 mA h g⁻¹ and a Coulombic efficiency of 98%. This enhanced electrochemical performance is attributed to the optimized electron density distribution and structural properties of CuO, which improve its effectiveness as an anode material.