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Atomic Scale Storage Mechanism Study of the Advanced Anode Materials for Lithium-Ion Batteries

Authors : Xi Wang, Yoshio Bando

Abstract : Lithium-ion batteries (LIBs) can deliver high levels of energy storage density and offer long operating lifetimes, but their power density is too low for many important applications. Therefore, we developed some new strategies and fabricated novel electrodes for fast Li transport and its facile synthesis including N-doped graphene-SnO2 sandwich papers, bicontinuous nanoporous Cu/Li4Ti5O12 electrode, and binder-free N-doped graphene papers. In addition, by using advanced in-TEM, STEM techniques and the theoretical simulations, we systematically studied and understood their storage mechanisms at the atomic scale, which shed a new light on the reasons of the ultrafast lithium storage property and high capacity for these advanced anodes. For example, by using advanced in-situ TEM, we directly investigated these processes using an individual CuO nanowire anode and constructed a LIB prototype within a TEM. Being promising candidates for anodes in lithium-ion batteries (LIBs), transition metal oxide anodes utilizing the so-called conversion mechanism principle typically suffer from the severe capacity fading during the 1st cycle of lithiation–delithiation. Also we report on the atomistic insights of the GN energy storage as revealed by in situ TEM. The lithiation process on edges and basal planes is directly visualized, the pyrrolic N "hole" defect and the perturbed solid-electrolyte-interface (SEI) configurations are observed, and charge transfer states for three N-existing forms are also investigated. In situ HRTEM experiments together with theoretical calculations provide a solid evidence that enlarged edge {0001} spacings and surface "hole" defects result in improved surface capacitive effects and thus high rate capability and the high capacity is owing to short-distance orderings at the edges during discharging and numerous surface defects; the phenomena cannot be understood previously by standard electron or X-ray diffraction analyses.

Keywords : in-situ TEM, STEM, advanced anode, lithium-ion batteries, storage mechanism
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