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Facet-dependent Rock-salt Reconstruction on the Surface of Layered Oxide Cathodes

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Abstract

The surface configuration of pristine layered oxide cathode particles for Li-ion batteries significantly affects the electrochemical behavior, which is generally considered to be a thin rock-salt layer in the surface. Unfortunately, aside from its thin nature and spatial location on the surface, the true structural nature of this surface rock-salt layer remains largely unknown, creating the need to understand its configuration and the underlying mechanisms of formation. Using scanning transmission electron microscopy, we have found a correlation between the surface rock-salt formation and the crystal facets on pristine $LiNi_{0.80}Co_{0.15}Al_{0.05}O_2$ primary particles. It is found that the originally $(01\bar{4})$ and (003) surfaces of the layered phase result in two kinds of rock-salt reconstructions: the (002) and (111) rock-salt surfaces, respectively. Stepped surface configurations are generated for both reconstructions. The (002) configuration is relatively flat with monoatomic steps while the (111) configuration shows significant surface roughening. Both reconstructions reduce the ionic and electronic conductivity of the cathode, leading to a reduced electrochemical performance.