

Abstract Submitted
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Lithiation of UHV-prepared CoO Conversion Battery Materials Studied by XPS and TEM¹ RYAN THORPE, Rutgers, SYLVIE RANGAN, ROBERT BARTYNSKI, MAHSA SINA, FREDERIC COSANDEY, Rutgers University — Lithium-ion conversion batteries can store 2-3 times more energy than intercalation batteries by fully reducing their constituent divalent or trivalent transition metal compounds during discharge. A prototypical conversion compound is CoO, which follows the reaction $2\text{Li}^+ + 2e^- + \text{Co}^{(2+)}\text{O} \rightarrow 2\text{Li}_2\text{O} + \text{Co}^{(0)}$ upon discharge. However, the cycling stability of conversion electrodes is poor, and capacity losses have prevented their implementation. To study the electronic and morphological changes that occur during the conversion reaction, we have grown 5 nm polycrystalline and epitaxial CoO films and exposed them to atomic Li in UHV to simulate cell discharge. Using XPS to monitor the valence state of Co and film stoichiometry, we find that at 25°C this reaction is inhibited by the formation of a Li₂O₂ overlayer, which is a kinetic barrier for Li diffusion. This is alleviated by heating the film to 150°C, thereby enhancing Li diffusivity through the overlayer and enabling complete reduction of the film. Epitaxial films are reduced with less Li than is required by polycrystalline films, suggesting the presence of channels through which Li is able to diffuse. In both cases, no cobalt phases other than CoO and Co are observed.

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