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Abstract title: Decoupling electrolyte and electrode reactions using *in-operando* electrochemical x-ray powder diffraction

Abstract text:

Lithium-ion batteries are the dominant energy storage technology – steady and significant progress toward lower costs, better safety, and better performance is being realized by an improved understanding and control of new materials and system engineering. Various novel materials for lithium-ion battery electrodes are emerging, most of which depend on alkali-metal alloys. Among them, aluminum electrodes offer the potential for high lithium-ion capacities at low costs, for example, capacities of 2000 mAh/g (six times higher than graphite, the current commercial standard) can be accessed at moderate temperatures (above 40 °C),[1] and aluminum foil electrodes can act as both the active material and current collector.[2] Nevertheless, challenges with capacity fade, electrolyte breakdown, slow diffusion and nucleation barriers still exist and alkali-metal electrochemical reactivity is not fully understood. Elevated temperature operation can be used to overcome nucleation barriers and slow diffusion, but at the cost of increased rates of electrolyte breakdown. Here, we combine controlled temperature electrochemical lithiation and delithiation with x-ray powder diffraction for in-situ studies of electrode and electrolyte reactions to shed light on these problems.

Our in-operando cell is based on commercially available ultra-high vacuum compatible Conflat flanges with beryllium windows and electrical feedthroughs to maintain commercially-relevant stack pressure and cell sealing.[3] We will report on cell design and mechanical, electrochemical, and diffraction performance, including full-powder-pattern refinement of the Li-Al electrode material during electrochemical lithiation and delithiation. Such refinement of the diffraction patterns allows us to quantify the fractions of the phases formed as well as details of the crystal structure (e.g. solid solution vs. new phase). The evolution of the measured cell potential and the powder diffraction pattern are shown in Fig. 1. We confirm the formation of AlLi, Al2Li3 and AlLi2 and follow their fractions in-operando during charge and discharge of the cell. Electrode composition from pattern refinement is compared to the composition predicted form electrochemical methods to separate the effects of electrode phase transitions and electrolyte breakdown, see Fig. 1a. Better understanding of phase formation in Li-ion battery electrode materials will enable more robust production and improved performance of the batteries on the market.

[1] M.Z. Ghavidel et al, Journal of The Electrochemical Society, 166 (16) A4034-A4040 (2019).
[2] H. Li et al, Nature Communications, 11, 1584 (2020).
[3] M.D. Fleischauer et al, Journal of The Electrochemical Society, 166 (2) A398-A402 (2019).

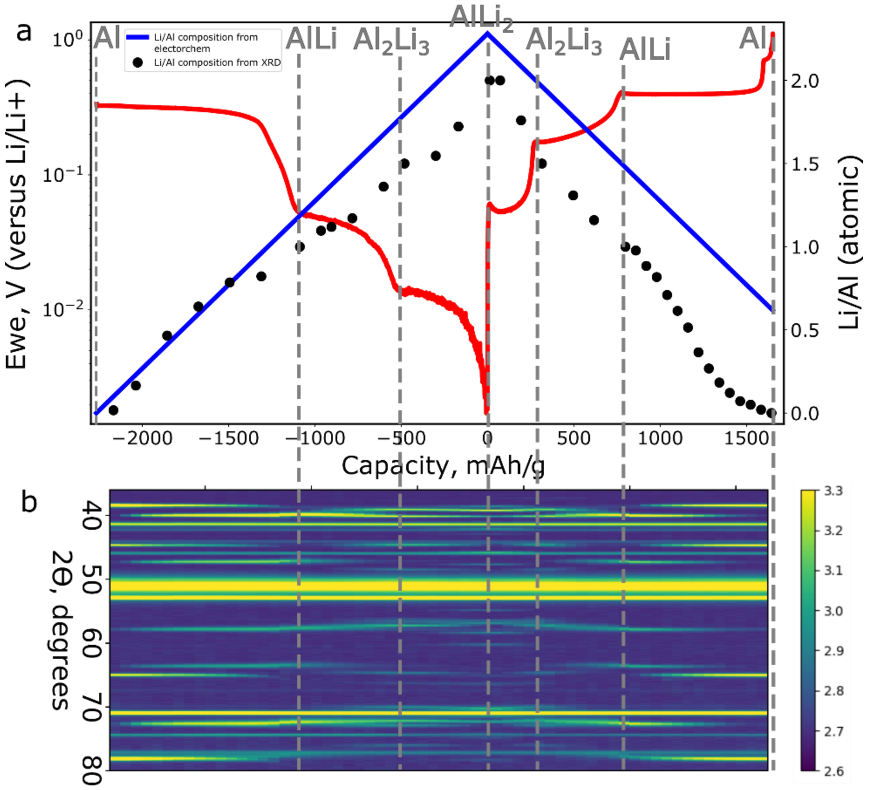

Fig. 1. The evolution of the (a) measured cell potential (red) and (b) the powder diffraction pattern during lithiation and delithiation. The apparent ratio of Li/Al via electrochemical (blue solid line) and x-ray pattern refinement (black dots) is also shown.