Quantifying slow diffusion in high capacity, multi-phase electrode materials

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Abstract text:

The use of metal alloys as negative electrode materials in lithium-ion batteries offers the potential for high lithium storage capacities at low cost, two key aspects for competitive energy storage technologies. Recent work shows that a single piece of aluminum foil can be used as both the negative electrode active material and current collector, and in a full cell configuration, support over 100 cycles without appreciable capacity fade.[1] This breakthrough is due to control of the nucleation and growth of the β-AlLi phase. Many other (higher capacity) Al-Li phases are predicted and can be detected when formed via thermal methods, but are generally not accessible via electrochemical methods. We demonstrated the reversible electrochemical formation of four Li-Al phases (β-AlLi, Al_2Li_3, $AlLi_{2-x}$, Al_4Li_9) by using slightly elevated temperatures to overcome nucleation and diffusion barriers.[2] There is a strong need to decouple kinetic (e.g. diffusion) and thermodynamic limits to understand and improve the practical performance of metal alloy electrodes.

Reliable quantification of diffusion rates can be challenging. Many of the techniques commonly used (e.g. potentio-or-galvanostatic titration, electrochemical impedance, cyclic voltammetry) depend on questionable assumptions or are not always applicable to materials with co-existing phases, as found in most lithium-metal alloys.[3] We will report on our use of the lithiation of aluminum foil as a model (i.e. diffusion limited) system to compare and contrast apparent (i.e. technique-dependent) lithium diffusion rates in the various Al-Li phases. In addition, as the samples are effectively planar, experimental diffusion measurements will be complemented with numerical simulations of one dimensional Fickian diffusion in the same conditions, to validate the calculated diffusion values against experimentally measured galvanostatic potential-capacity data sets.

All electrochemical experimental data was collected using Conflat-style electrochemical cells, which we designed for repeatable electrochemical testing over a wide temperature range (30 - 150◦C).[4] Repeatability is enabled by engineered alignment of electrodes, adjustable control of stack pressure, and ultra-high vacuum tight Conflat seals. Cell-to-cell variability (including all factors) is <5% at intermediate temperatures (<90◦C) and <10% at higher temperatures (120-150◦C) as we approach the limits of liquid electrolyte stability and the melting point of Li (181◦C). Galvanostatic data was collected over a wide range of current densities (from dynamic to near-equilibrium rates, e.g. C/10 to C/280) and a wide range of tightly controlled temperatures (30 +/- 1 to 150 +/- 3 °C). Examples of the dramatic

effects of current density and temperature on phase formation / cell potential and final capacity are provided in the attached figure. Insight in to technique-dependent diffusion measurements and robust estimates of diffusion coefficients validated against a broad experimental data set will improve our analysis of, and the potential for, metal alloy electrode materials.

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[2] M.Z. Ghavidel et al., Journal of The Electrochemical Society, 166 (16) A4034-A4040 (2019).
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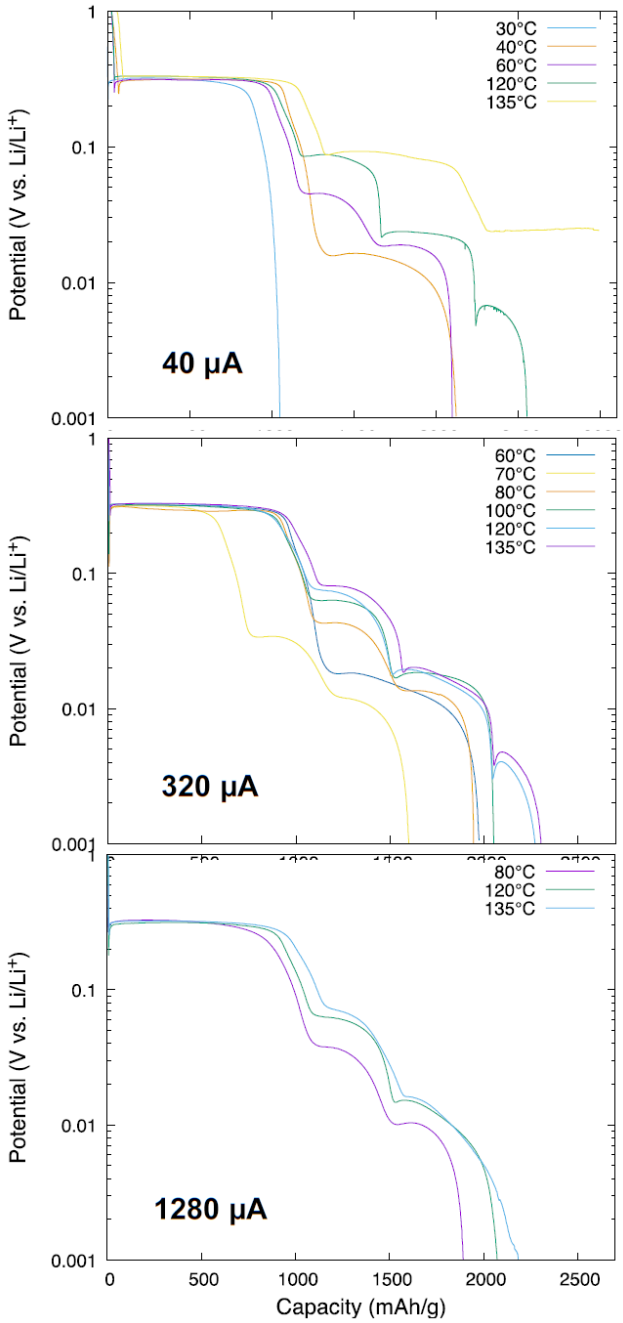

Figure 1. Potential vs. capacity data for a variety of currents and temperatures.