

Kinetic Study of the Reversible Lithiation in Si Thin Film Anodes

J. Miao, C. V. Thompson.

Sponsorship: Singapore-MIT Alliance for Research and Technology, Skoltech Center for Electrochemical Energy Storage

Among all the known anode materials for Li-ion batteries, Si is a promising candidate for applications in CMOS-compatible microbatteries. It has extraordinarily high capacities (8375 Ah/cm^3 , 3579 Ah/kg), which is a result of the unique alloying mechanism during lithiation that involves bond breakage and a series of formation of new short-range structures. The reversible lithiation of Si anodes (Figure 1, highlighted) has not been extensively studied, and there have also been debates over whether it is a diffusion process or a phase-transition process. Here we adopt the potentiostatic technique to study the reversible phase transitions that occur in the second and subsequent lithiation cycles.

It was found that there is always a peak in the current vs. time curve under desirable potentiostatic test conditions in the reversible lithiation regime (Figure 2). The existence of the peak suggests there is phase transition in the reversible lithiation, rather than pure diffusion where current should decrease monotonically with time. The time at which the peak occurs (t_{peak}) increases with the applied potential, which indicates slower kinetics for the phase transition. Kinetic parameters could be extrapolated from the current vs. time curves upon modelling and fitting.

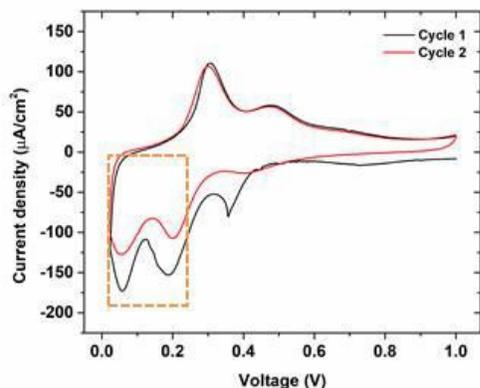


Figure 1: CV (cyclic voltammogram) curves in the first and second cycles of a LiPON-coated Si thin film sample. The highlighted voltage regime indicates the reversible lithiation regime, The scan rate is $40 \mu\text{V/s}$.

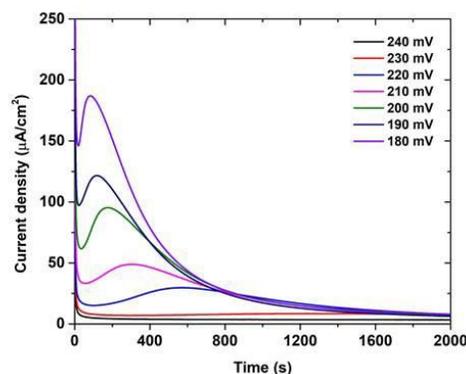


Figure 2: Current vs. time curves at different voltages (180, 190, 200, 210, 220, 230, 240 mV, respectively) after a potentiostatic hold at 270 mV for 4.5 hours in a LiPON-coated Si thin film sample (180 nm thick).

Further Reading

Miao, J., & Thompson, C. V. (2018). Kinetic Study of the Initial Lithiation of Amorphous Silicon Thin Film Anodes. *Journal of the Electrochemical Society*, 165(3), A650-A656.