Insight into Electrochemical Characteristics of Si and C-coated Si Particulate Electrodes for Lithium Ion Battery

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Being an anode for Li ion battery, Si possesses a maximum Li uptake of Li$_4$Si, corresponding to a theoretical capacity of 4200 mAh/g. The Si anode application has nevertheless been hindered by rapid capacity decay upon cyclic charge/discharge. Although it has generally been suggested that the poor cycle life is mainly associated with volume variations upon Li alloying/de-alloying, current understanding of the mechanistic mechanism to such failure in fact remains vague, and the interplay between the architecture of a particulate Si electrode and its cycle life has not been systematically explored. In addition, information related to other basic electrochemical characteristics of this anode material is even scarce. This is partly because it has indeed been difficult to achieve long enough cycle life for detailed characterization.

By optimizing some of the electrode architecture factors, including particle size and conductive additive content, particulate electrodes containing either Si or C-coated Si particles have been managed to exhibit cycle life of several tens cycles with >90% capacity retention and a charge depth as high as 1000 mAh/g-Si (Fig.1). The electrochemical characteristics of these electrodes have thus been systematically studied by impedance spectroscopy (Fig. 2), cyclic voltammetry (Fig. 3), and charge/discharge test, in conjunction with structural study using in-situ synchrotron XRD (Fig. 3). This work will present the experimental results that not only provide essential understanding on the electrochemical behaviors of Si itself, but also have revealed several novel effects of the C-coating on Li alloying/de-alloying kinetics of Si particles.

Fig. 1. Cycle life tests for C/Si (1000 mAh/g-Si) and Si (600 mAh/g-Si) electrodes. Open symbols are charging capacity, and solid symbols are discharging capacity.

Fig. 2. AC impedance spectra for fresh Si and C-coated Si electrodes.

Fig. 3. In situ synchrotron XRD patterns of Si upon charging.