Nanostructured Si-Based Negative Electrodes for Li-ion Batteries

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The use of Si alloy negative electrodes in practical high energy density Li-ion cells has now been well-established [1]. Their successful implementation requires combining materials, binder, coating, electrolyte and cell design. This presentation will focus on recent advances in Si alloy materials.

Optimization of Si alloys requires a detailed understanding of the interaction of Si with other active and inactive phases. We have found that internal stresses can develop between active Si and an inert inactive phase can be as high as 2 GPa during lithiation, and can shift the voltage curve of Si by hundreds of mV [2], as shown in Figure 1 below. This voltage shift can result in the $Li_{15}Si_4$ formation peak, which usually resides at about 50 mV [3], to be shifted below 0 V, thus inhibiting $Li_{15}Si_4$ formation. Moreover, the stress induced voltage shift can cause a significant portion of the Si lithiation voltage curve to be shifted below zero volts, resulting in capacity reduction [2]. Different inactive phases were found to shift the Si voltage curve by different amounts, implying that the interaction between Si and inactive phases can vary substantially, depending on composition [4]. Such results have important implications regarding the design of new alloy materials.

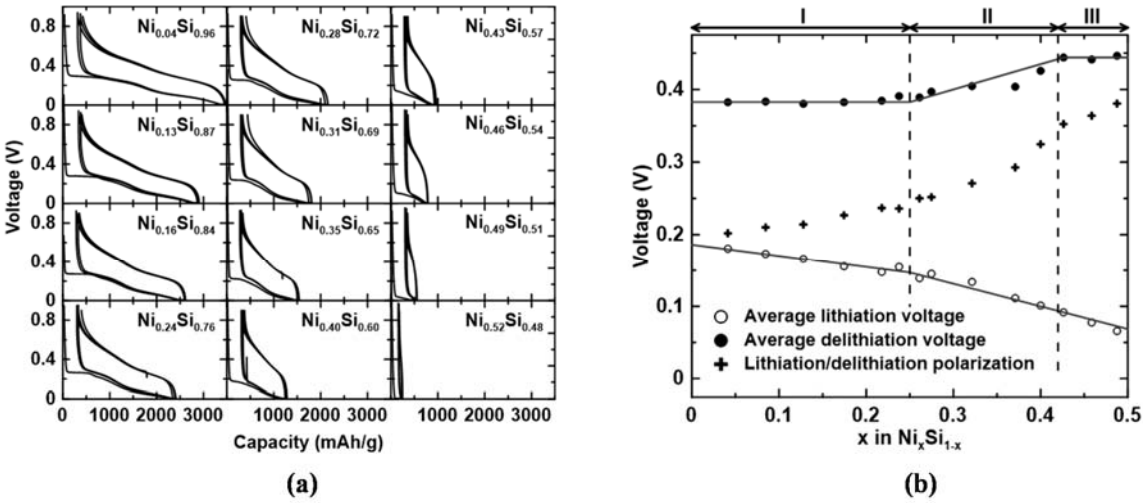

Figure 1 (a) The voltage curves and (b) the average lithiation and delithiation voltages of Ni_xSi_{1-x} alloys as a function of composition. Reproduced with permission from Reference 2.

References

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