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Reversible Cycling of Silicon and Silicon Alloys[1]

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Lithium ion batteries typically use a graphite negative electrode. Silicon can store more lithium than any other element and has long been considered as an attractive replacement for graphite. The theoretical lithium storage capacity of silicon is nearly ten times higher than graphite volumetrically and three times higher gravimetrically. The equilibrium Si-Li binary system is well known. Completely new phase behaviors are observed at room temperature. This includes the formation of a new phase, Li15Si4, which is the highest lithium containing phase at room temperature [1]. The formation of Li15Si4 is accompanied by a 280 percent volume expansion of silicon. During de-alloying this phase contracts, forming amorphous silicon. The volume expansion of alloys can cause intra-particle fracture and inter-particle disconnection; leading to loss of cycle life. To overcome issues with volume expansion requires a detailed knowledge of Li-Si phase behavior, careful design of the composition and nanostructure of the alloy and the microstructure of the negative electrode [2]. In this presentation the phase behavior of the Li-Si system will be described. Using this knowledge alone, strategies can be developed so that silicon can be reversibly cycled in a battery hundreds of times. Further increases in energy density and efficiency can be gained by alloying silicon with other elements, while controlling microstructure [2]. Coupled with negative electrode design strategies, practical negative electrodes for lithium ion cells can be developed based on bulk materials, with significant energy density improvement over conventional electrodes.

[1] M.N. Obrovac and L.J. Krause, J. Electrochem. Soc., 154 (2007) A103.

[2] M.N. Obrovac, Leif Christensen, Dinh Ba Le, and J.R. Dahn, J. Electrochem. Soc., 154 (2007) A849

[1] Reversible Cycling of Silicon and Silicon Alloys