

# A New Synthetic Route for $\text{Si}_{1-x}\text{O}_x$ : Microstructure, Thermal Stability and Electrochemistry

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$\text{Si}_{1-x}\text{O}_x$  is a promising Li-ion battery negative electrode material because of its high capacity and unique microstructure that leads to good cycle life<sup>[1,2]</sup>. However, SiO is typically made by high temperature methods that are difficult to realize, especially at lab scale. Ball milling Si + SiO<sub>2</sub> has also been used to prepare SiO, however the microstructure is inferior to commercially made materials. Here,  $\text{Si}_{1-x}\text{O}_x$  negative electrode materials with different oxygen content were prepared using a new convenient and scalable method. The preparation method allows efficient control of oxygen content and results in a similar microstructure as commercially purchased SiO. This allows for detailed study of the microstructure, cycling performance and thermal stability of  $\text{Si}_{1-x}\text{O}_x$  with different oxygen contents. XRD and TEM results show that the samples are composed of nanocrystalline Si embedded in an amorphous SiO<sub>x</sub> matrix. The differential capacity curves (Figure 1(a)) of  $\text{Si}_{1-x}\text{O}_x$  show that Li<sub>15</sub>Si<sub>4</sub> formation is fully suppressed when the oxygen content is increased to around 20 mol.%. A peak during the first lithiation step was found to be directly related to oxygen content. The average lithiation voltage and the peak area change accordingly with the oxygen ratio in the samples. Some of the samples synthesized by this new route exhibit better cycling performance at higher capacities (Figure 1(b)) compared to commercially obtained silicon monoxide (Si<sub>0.51</sub>O<sub>0.49</sub>). The volumetric capacity of the alloys are larger than 2000 Ah/L. This performance would correspond to a 33% increase in volumetric energy compared to a baseline LiCoO<sub>2</sub>/graphite cell<sup>[3]</sup>.

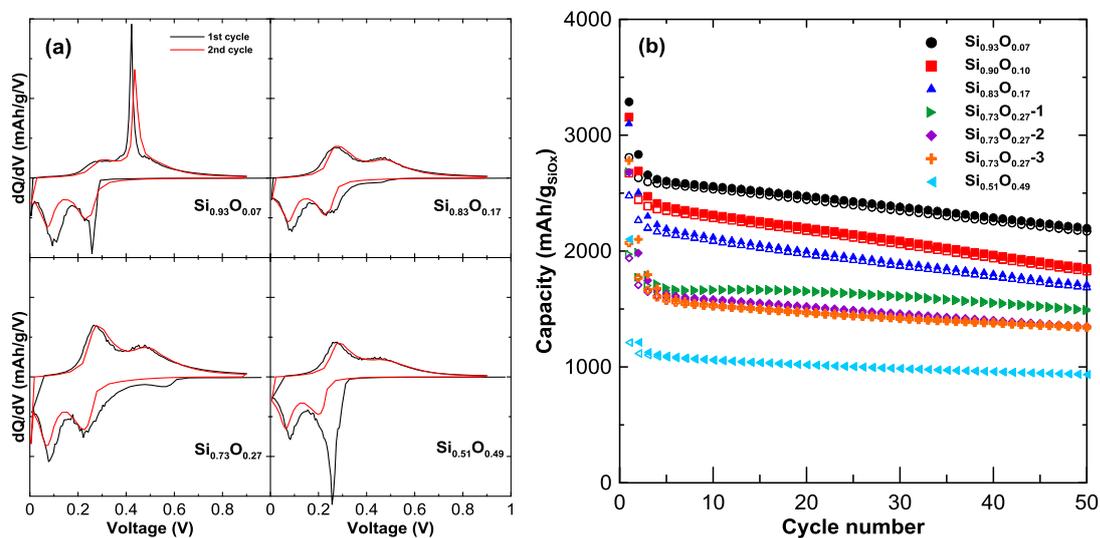


Figure 1 (a) Differential capacity curves and (b) Cycling performance of  $\text{Si}_{1-x}\text{O}_x$  alloys

## References:

- [1] Y. Hwa, C. M. Park, and H. J. Sohn, *J. Power Sources*, **222**, 129 (2013).
- [2] X. Zhao, R. J. Sanderson, M. A. Al-Maghrabi, R. A. Dunlap, M.N. Obrovac. *J. Electrochemical Soc.*, **164** (6) A1165-A1172 (2017).
- [3] M. N. Obrovac, and V. L. Chevrier, *Chem. Rev.*, **114**, 11444–11502 (2014).