

Silica as anode precursor for lithium ion batteries

M. Schrandt^a, P. Kolla^a, W. Rhine^b, R. Cook^c, and A. Smirnova^{a,d}^aMaterials Engineering and Science Program, South Dakota School of Mines and Technology, Rapid City, SD 57701^bAspen Aerogels, Northborough, MA 01532^cZyvex Technologies, Rapid City, SD 57701^dDepartment of Chemistry and Applied Biological Sciences, South Dakota School of Mines and Technology, Rapid City, SD 57701

In lithium ion batteries, Si-based anodes possess the highest specific capacity from four to 10 times greater than graphite^{1,2}. However, up to 400% volume expansion of Si during lithiation results in anode pulverization due to mechanical stresses. The goal is to develop silicon-based anode that can withstand lithiation-delithiation cycles without mechanical degradation. The major steps including silica synthesis, polymer templating, and magnesium vapor reduction will be discussed.

To avoid mechanical degradation of silicon, the critical value of the silicon particle size/wall thickness should be below the required threshold of <50nm^{3,4}. Thus, it is crucial to maintain the silicon particle size in this range. The second major requirement for silicon anode in lithium ion batteries is to have the second conductive phase, e.g. graphite or graphene, in the form of a flexible coating that can withstand lithiation-delithiation without deterioration of the carbon phase.

Two types of silicon oxide precursor materials that meet these requirements have been evaluated, among them hollow silica microspheres from 3M and silica aerogel from Aspen Aerogels. Preparation of Si precursor materials has been performed by (1) Mixing with resorcinol-formaldehyde (RF) monomer solution; (2) Performing magnesium reduction; and (3) Removal of unnecessary impurities such as magnesium oxide by washing the material in 0.1M HCl.

The SEM, TEM, EDS, cyclic voltammetry performance, cycleability, charge-discharge profiles, and XRD patterns after different number of lithiation-delithiation cycles will be discussed.

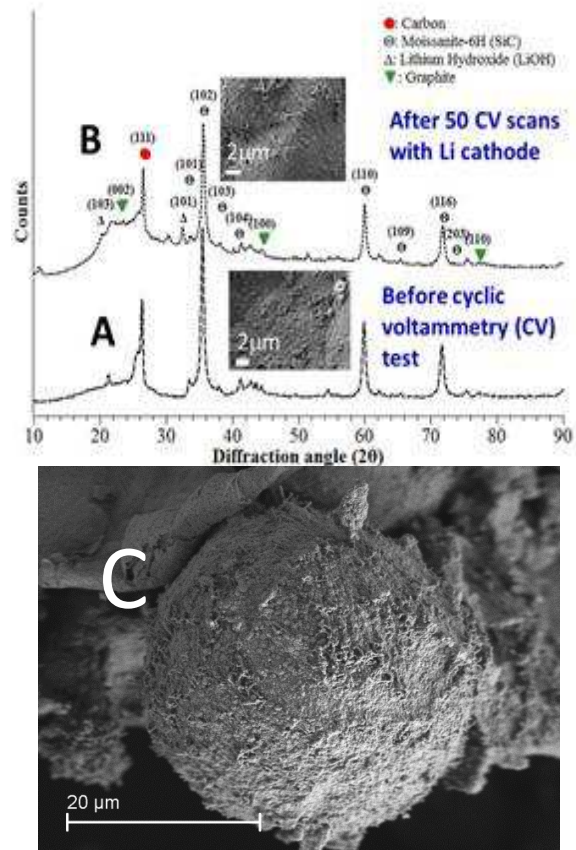


Fig. 1: XRD data for carbon-coated Si spheres from 3M produced by Mg reduction of SiO₂. (A) Before cyclic voltammetry;

(B) After 50 cycles; (C) Silicon sphere with ~10nm carbon coating after Mg reduction RF templated SiO₂.

References:

- ¹ A. Kraytsberg, Y. Ein-Eli, J. of Power Sources, **196**, 886 (2011).
- ² W. J. Zhang, J. of Power Sources, **196**, 13 (2011).
- ³ X. H. Liu, L. Zhong, S. Huang, S. X. Mao, T. Zhu, J. Y. Huang, ACS Nano, **6**, 1522 (2012).
- ⁴ U. Kasavajjula, C. S. Wang, A. J. Appleby, J. of Power Sources, **163**, 1003 (2007).