Structure-Property Relationships of Silicon Nanoparticles Produced by Free Space Silane Pyrolysis

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Silicon continues to attract significant research and development attention as a negative electrode material for next-generation lithium-ion batteries [1]. To counteract the high volume expansion associated with lithiation, silicon nanoparticles are one materials engineering approach to extend cycle life. However, silicon nanoparticles can be synthesized using multiple routes, instruments, and parameters. Correlating morphology and size with battery properties is needed to unify the diverse knowledge of these different approaches and provide predictable tunability of nanoparticle properties. In our work, we discuss the structure-property relationship of silicon nanoparticles pyrolyzed from silane gas and correlate size distribution, morphological characteristics, and agglomeration with electron microscopy, *in situ* optical spectroscopy, and battery performance. Silicon nanoparticles from Alfa-Aesar with a reported average particle size of 50 nm or less actually contain particles ranging from 20 to 200 nm while those produced at Institutt For Energiteknikk (IFE) are consistently less than 100 nm and have a narrower size distribution. Although they have similar performances, the narrower size distribution of IFE silicon nanoparticles could have beneficial consequences for pre-lithiation and the uniform application of coatings used to suppress volume expansion upon silicon lithiation. With the breadth of silicon nanostructures being studied today, a common knowledge base of structure-property relationships, methods to measure and tune them, and their impact on advanced and complex modifications is important for progression of the broader field.

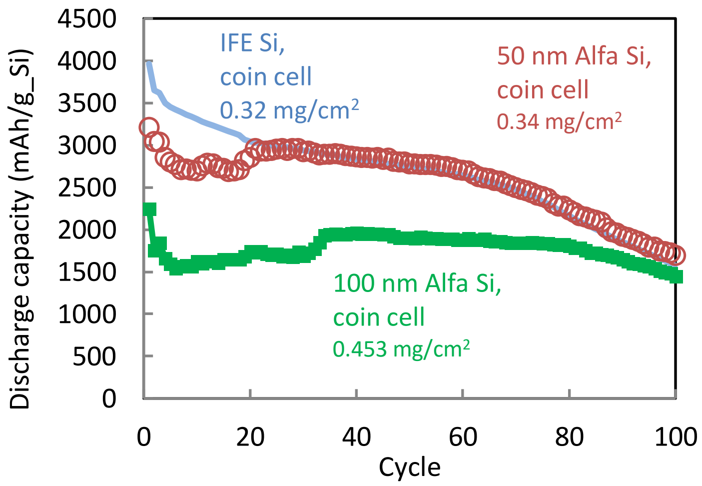

Figure 1. Coin half cell cycling of different types of silicon nanoparticles at 0.358 A/g.

References:

[1] M. Ashuri, Q. He, and L. L. Shaw, "Silicon as a potential anode material for Li-ion batteries: where size, geometry and structure matter," *Nanoscale*, vol. 8, pp. 74-103, 2016.