

Post mortem investigation of the chemical environment in silicon-based lithium-ion batteries by XRS

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Lithium ion batteries are one of the best solutions for energy storage firstly due to the lighter weight of the lithium conferring high energy density. This also enables the flexibility in design and the portability that facilitates the use in several applications ranging from mobile devices to automobile market. In the research for materials that can reversibly host or release large quantities of lithium ions, it has been realized that silicon offers interesting possibilities because of its high theoretical capacity (3579 mAh/g) and natural abundance, compared to the usual commercial electrode, graphite (372 mAh/g). However, silicon suffers large volume expansion upon the insertion-disinsertion of the lithium ions, which results in the continuous formation of solid electrolyte interphase (SEI), leading to Li trapping and capacity loss. This continuously happen, leading to irreversible capacity and electrical contact loss [1].

One way of limiting volume expansion is using silicon nanoparticles, where the small size enables Li transportation and strain relaxation. These nanoparticles can also be embedded into a matrix to form a composite electrode. Using composites can mitigated volume changes, therefore reducing the capacity loss. However, the changes on the chemical environment of the composite and nanoparticles silicon based-electrodes are not well known.

We investigated the variations of the chemical environment in fresh and aged Silicon-anodes by XRS, in particular to study the formation and composition of the SEI in function of the materials morphology (e.g. NPs versus composite, see **Fig 1. a. & b.**) and state of charge (lithiated and delithiated states after typically few cycles and/or long-term cycling). XRS experiments were performed on ID20 at the ESRF on reference samples (pure compounds) and electrodes in specially designed airtight cell. We scanned the energy at the edges of C, O, F, Li and Si. The analysis of the spectra allowed us to observe qualitatively the formation of organic and inorganic species during cycling, and a quantitative attempt to deconvolute the spectra based on available references was performed to extract the amount of species on the SEI (see **Fig 1. a. & b.**).

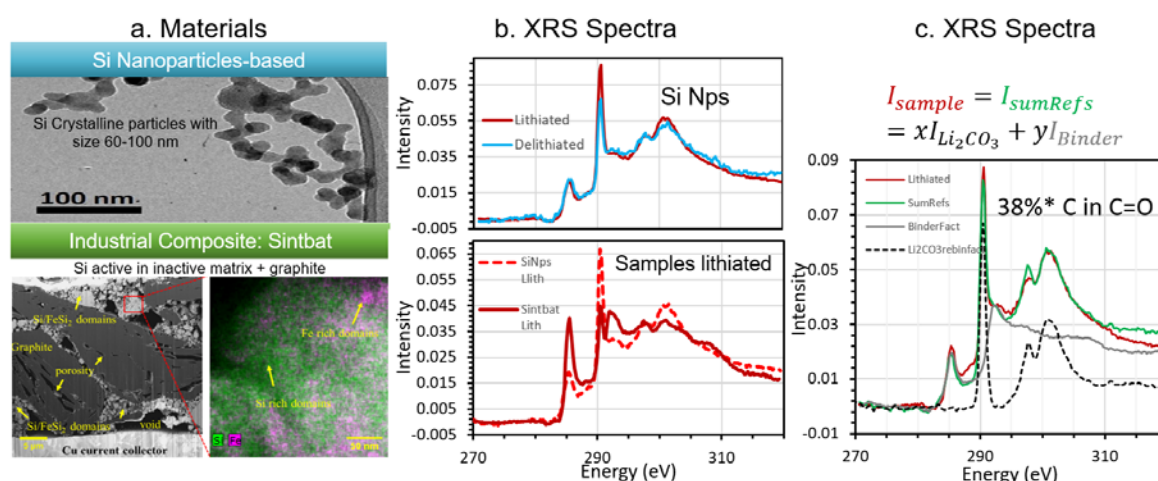


Figure 1: a. Materials investigated. b. Data obtained in the electrodes at different states. c. Analysis using references

References

[1] - X. Zuo et al. Nano Energy 31, 113 (2017).