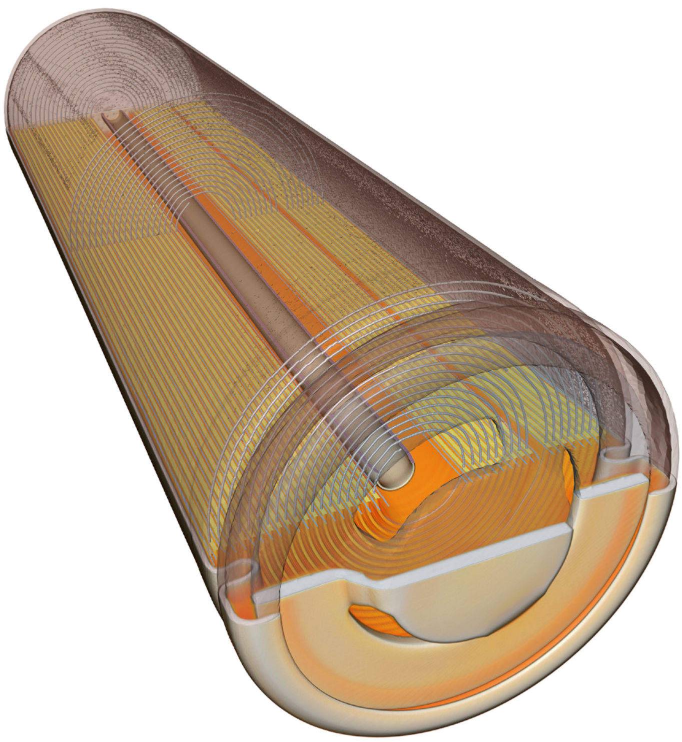
thermo scientific

APPLICATION NOTE

Multiscale 3D Imaging Solutions for Li-ion Batteries

The increasing demand for electric vehicles and consumer electronics in recent years has caused Li-ion batteries to attract significant attention due to their high energy and power density compared to other commercial rechargeable battery technologies. In order to further advance Li-ion battery technology for better performance and to increase safety, a fundamental understanding from materials chemistry to battery structure is essential.



Introduction

One of the biggest challenges to understand Li-ion battery technology is its intrinsic 3D multiscale nature. The battery needs to be characterized from cell level (mm length scale) to particle level (nm length scale) in three dimensions. In this application note, we present a multiscale 3D imaging and analysis workflow that enables quantitative understanding of the structure-performance relationship in Li-ion batteries.

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Characterization at the cell level

MicroCT is the enabling technology that allows for imaging large volumes at the mm scale with µm resolution. Researchers and engineers are interested in using this technique to characterize batteries at the cell level. **Figure 1** shows a 18650 battery cell imaged in 3D with the Thermo Scientific™ HeliScan microCT to better understand the cell structure evolution during cycling. The quantitative analysis of the current collector position before and after cycling indicates the electrode volume expanding during cycling. These insights can be used to correlate with battery degradation phenomena.

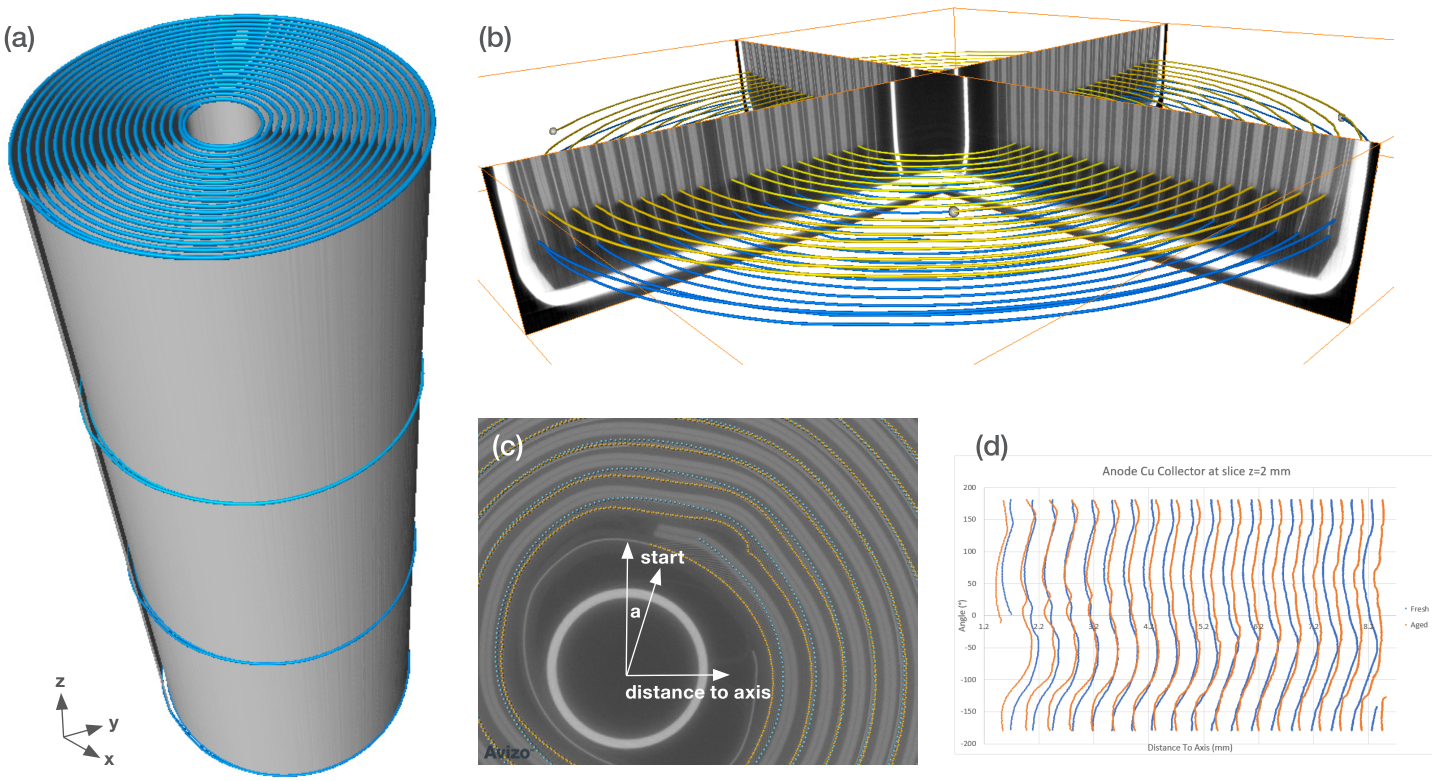


Figure 1. 3D imaging analysis on an 18650 Li-ion cell. Blue represents the fresh cell and yellow represents the cycled cell; (a) 3D reconstruction of the Cu current collector in the 18650 cell (fresh state); (b) Overlay of the Cu current collector of fresh and cycled battery in 3D; (c) 2D image (XY plane) of the fresh and cycled cell with Cu current collector extracted and overlay at center area; (d) Quantitative comparison of the Cu current collector position between fresh and cycled cell

Characterization at the electrode level

At the electrode level, the Thermo Scientific™ Helios PFIB DualBeam enables researchers and engineers to generate a representative volume (>100 µm field of view) with nm resolution and high-throughput materials milling. The 3D volume can then be further used in microstructure quantification for structure-performance analysis as well as a 3D template for modeling and performance prediction. **Figure 2** shows the cross-sectional image of a NMC cathode and a graphite anode at 100 µm and 125 µm horizontal field of view respectively.

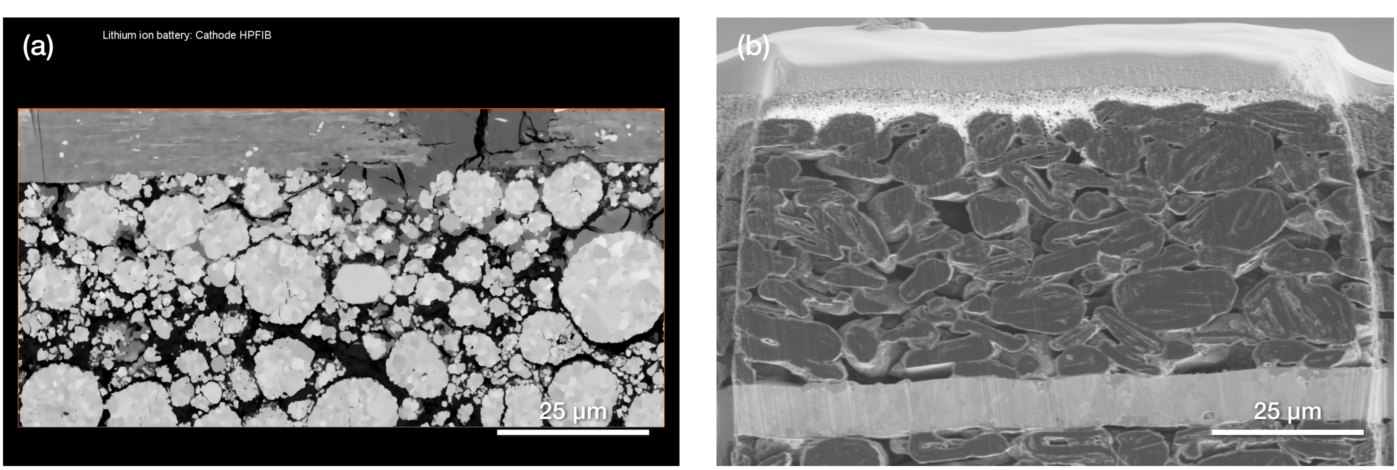


Figure 2. 3D imaging of Li-ion battery electrode with Helios G4 PFIB DualBeam. (a) Cross-sectional view of the NMC cathode; the field of view is 100 µm; (b) Cross-sectional image of graphite anode, 125 µm field of view.

Figure 3 shows a 3D reconstruction of a SiO/C anode by using low kV EDS mapping. The silicon particles in the anode can be seen to have a CMC coating, which is applied to make them more resistant to cycling degradation. This 3D reconstruction was obtained using a Thermo Scientific Scios DualBeam.

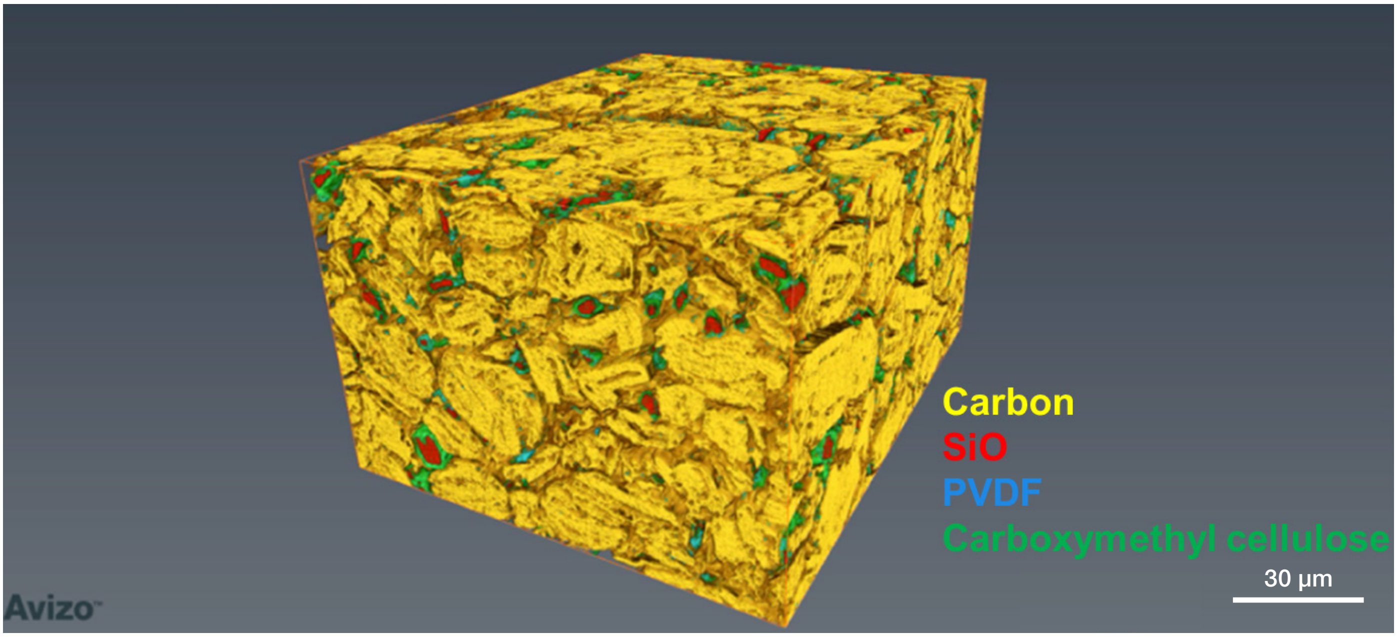


Figure 3. 3D EDS mapping of SiO/C anode.

Elemental analysis

One challenge of using EDS for elemental analysis is to detect lithium within the electrode/particle, which is critical for electrode materials property analysis. With a time-of-flight secondary ion mass spectrometer (TOF-SIMS) in the DualBeam system, direct imaging of lithium in the cathode structure can be achieved. **Figure 4** shows the 3D reconstruction of the lithium distribution within an NMC cathode.

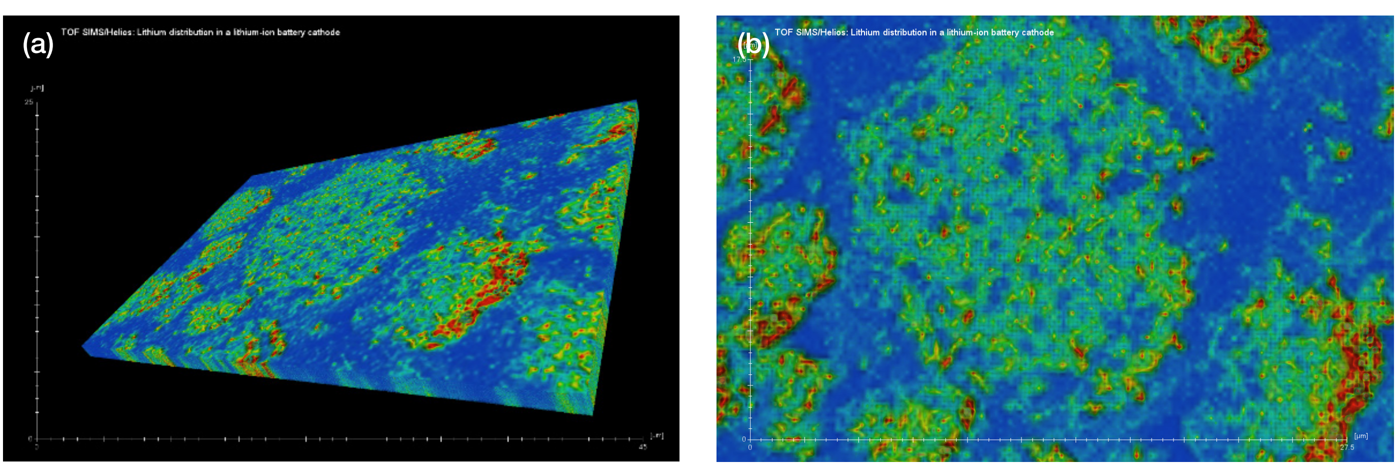


Figure 4. (a) 3D lithium (^{7}Li isotope) distribution within the NMC cathode; 3D reconstruction volume of 40 µm x 26 µm x 1.25 µm (x*y*z).
(b) Enlarged SIMS map of a 2D slice showing Li distribution within NMC particles.

DualBeam systems also provide detailed chemical and elemental analysis at the electrode particle level. **Figure 5** shows the analysis of a single NMC particle in 3D. Images at different depth are taken in the Scios DualBeam. By milling the particle and taking images at different depth of the particle, high resolution images of the microstructure within the particle are collected. The different contrasts present in the primary particles may indicate chemical composition or crystallographic differences and can be further analyzed by EDS, SIMS, and EBSD techniques available in the DualBeam.

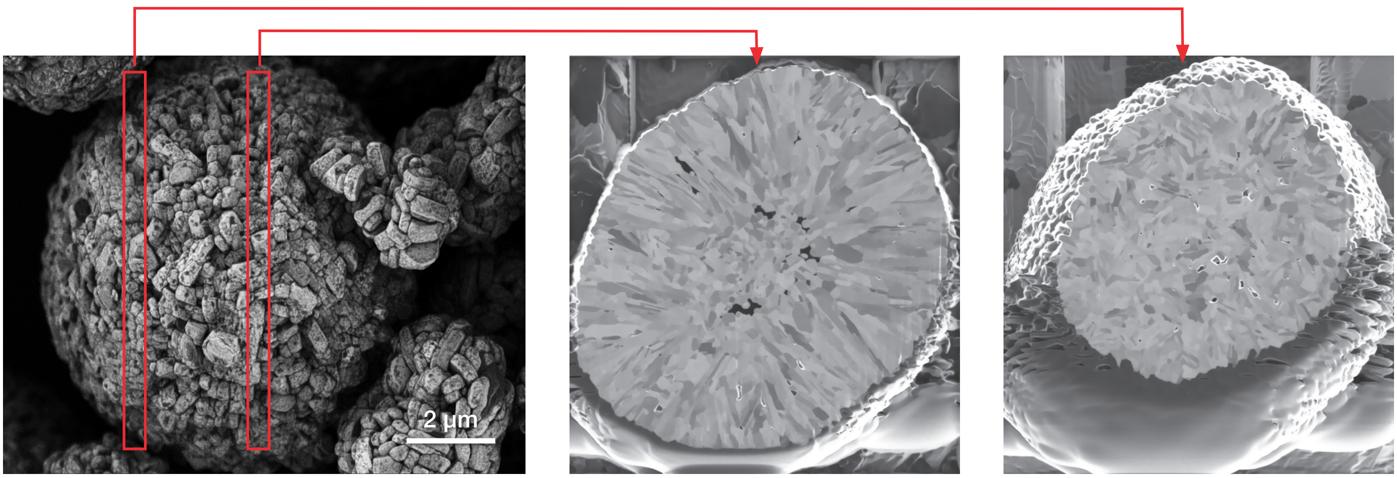


Figure 5. Imaging analysis of Li-ion battery electrode particle via DualBeam. Cross-sectional view of the individual NMC particle at different depth.

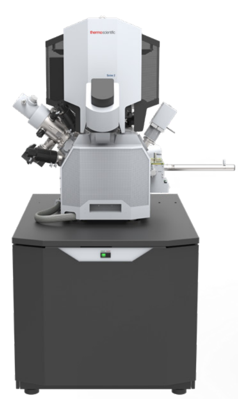
Conclusion

Understanding the structure-performance relationship in Li-ion batteries at different stages in the lifecycle requires imaging and analysis at multiple length scales and in 3D. Geometric parameters such as volume fraction, surface area, particle size distribution, and tortuosity are typically assessed using a combination of microCT and FIB-SEM techniques. Thermo Fisher Scientific provides a complete workflow of microCT and DualBeam systems with advanced accessories and software suites that provide a complete understanding of the battery at multiple scales and in 3D, ultimately enabling researchers and engineers to develop better performing, safer batteries with longer lifetimes.

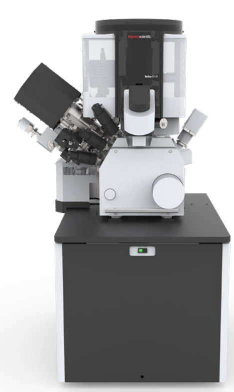
Related products

HeliScan microCT

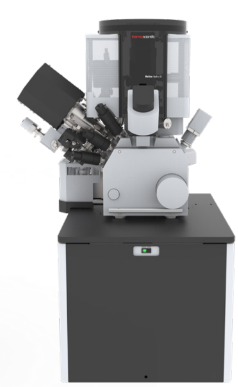
Scios 2 DualBeam



Helios G4 PFIB DualBeam



Helios Hydra DualBeam



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