Better Batteries

An insight into the inner life of simple AAA batteries reveal aspects for their aging process in order to make these last longer.

INTRODUCTION

Lithium based batteries is the dominant battery technology for household and portable items. Due to their high specific energy and energy density, they can be built lighter and smaller than other battery types. Researchers are trying to understand mecha-nisms behind degradation, capacity loss or charging speed, but are slowed down by suboptimal experi-mental techniques lacking physicochemical insights. Together with the industry partner FINDEN LTD, DESY offers a non-invasive 3D imaging technique that allows identification of the chemical composition at the micrometer scale in operando studies.

CHALLENGE

Lithium based batteries, used for cars or household items, become more and more prominent due to their high energy density and the resulting electrochemical properties. Several chemical reactions happen in battery during use and as the consequence the micrometer scaled heterogeneities form.
These heterogeneities are known to be starting point of material degradation and hence significant performance loss.
Imaging the heterogeneities with synchrotron radiation x-ray computed tomography (SR-μCT), a standard 3D non-invasive imaging technique, is nearly impossible, because the image contrast is produced by element specific x-ray absorption, which is low for most chemicals inside batteries.
If conducted, standard x-ray tomography can only produce greyscale images, from which it is difficult to draw conclusions about reactions relevant for performance losses or safety concerns.
Any reaction inside the battery will change the chemical composition of the battery and any novel approach should be able to observe the changes. A way to do this, is by using x-ray diffraction computer tomography (XRD-CT). This technique does not rely on the absorption of incident x-rays, but on the electron density of the sample. Synchrotron x-ray radiation can then be used to investigate samples with low x-ray absorption materials as one find in a battery. Another important aspect is the possibility to study batteries in different charging levels and examine the dynamics inside the battery during use.
Lithium ion batteries have many advantages over other batteries types like nickel-based batteries, such as no memory effect, higher power and energy density. These advantages are the reason many people bet on LIB to be an important part in the storage of renewable energy to balance the variable power output of renewable energies. This strengthens the need for an experimental technique that allows for time resolved in operando studies on commercially available devices, because they differ from their lab counterparts.

Simple AAA batteries, almost a staple in any household, office or organization: How can we make them to last longer? A look inside the batteries might get us a step closer to a more efficient and sustainable of these everyday helpers.

Finden

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METHOD

For any XRD-CT scan a monochromatic narrow x-ray beam, called pencil beam, is positioned on the sample and the area detector is positioned in transmission geometry. The data acquisition technique used here is a zig-zag scan. Here 2D diffraction patterns are collected at each translation step for each rotation step. Followed by an integration over the azimuthal angle and reorganized in sinograms.

For this case study scientist performed noninvasive x-ray diffraction computer tomography on commercially available AAA type batteries at the beamline P07 experimental hutch 2 at PETRA III on the DESY campus in Hamburg. Over 750,000 diffraction patterns were collected and the automated data processing used the Rietvield algorithm to reconstruct 3D images.

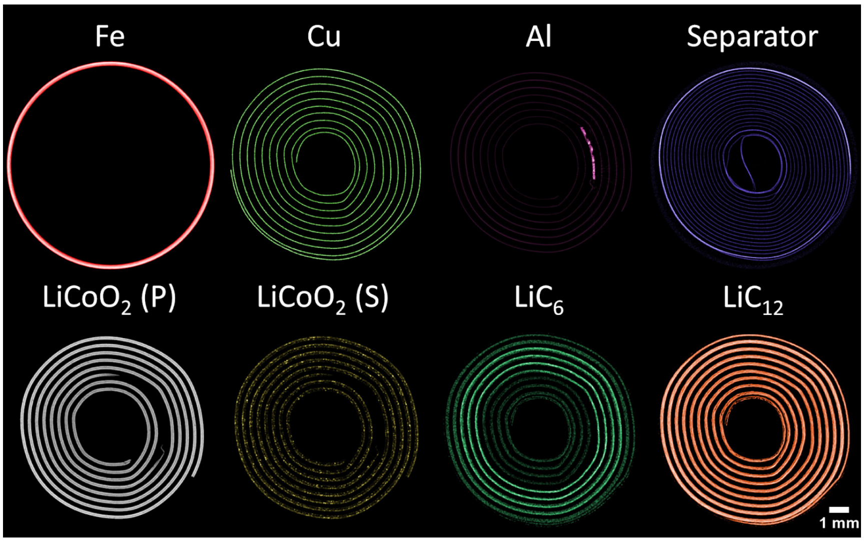

Figure 1: Selected chemical phases in a Lithium ion battery. Top row: iron hull, copper and aluminum current collector, organic separator. Bottom row: Cathode materials and anode materials.

INSIGHTS AND ANALYSIS

Slices from an AAA-type LIB colored by the amount of a certain chemical compound are shown in fig1. As one can see, the chemical composition is subtracted from the diffraction data and can be presented in vivid figures. In the top row the iron case, the copper collector and the organic separator can be identified, as well as the rolled-up layer structure of the battery. In the bottom row on the left side the cathode material, Lithium cobalt oxide ($LiCoO_2$), is colored. The (s) and (p) indicate different different components of the electrode. On the bottom left side, the anode material, Graphite is shown. Lithium ions intercalated between the graphite layers and form the phases LiC_6 and LiC_{12}.
The LiC_6 phase has an heterogenous distribution and is mainly distributed in the inner layers. To enhance the battery capacity and speed up the charging process, one can tackle this non-uniform phase distribution.
If not limited by a 2D representation, a full 3D model can be created. Although batteries consist mainly out of low z-materials, the XRD-µCT was able to produce meaningful data. The reason is, that XRD-CT produces diffraction patterns, which contain various information about crystal phases, like crystal structures, degree of crystallinity or crystal sizes. From this information it is also possible to identify the local chemical composition, to follow the formation of heterogeneities and track the diffusion of phases through the battery. A clever trick also enhances data quality by analyzing each voxel by its own. In each voxel fewer crystalline phases are present and the relative detected intensities of each phase is increased and hence the data quality is improved. As a consequence, chemical phases were detectable down to 1% of weight. This helps especially for samples with similar chemical phases, i.e. lithium graphite intercalation compounds LiC_6 and LiC_{12} at the electrode of LIB.
In addition, the LIB can also be cycled between measurements, meaning it will be charged and discharged under well defined conditions. With this setup long term studies of for example the degradation of the LIB performance is possible.

BENEFITS

XRD-CT proved to be a great extension for standard x-ray CT as it delivered information of chemical composition with micrometer spatial resolution and revealing unwanted phases and non-uniform phases distribution. XRD-CT can be applied to real life battery and other devices, making it extremely useful for industrial clients with specific needs and problems. This method can be applied under time resolved conditions, to examine phases transformation inside a battery while charging or discharging the battery. Another interesting aspect is the imaging of the ageing process, to observe mechanical damage on the structure and link it to their starting points at the micrometer scale, by scanning the battery after various amounts of charging cycles. Also, XRD-CT showed its possibilities in depth resolution, which is very important for industry clients that want to do research on actual devices they are aiming to improve. With the ultra-high spatial resolution of synchrotron radiation XRD-CT provided by PETRA III is ready to help industrial clients on their way to understand reasons for battery ageing, reduced capacities and slow charge cycles.
The research on LIBs is far from being concluded. Especially the research on electrodes design and materials holds room for improvements. Other lithium-based battery types, i.e. Lithium-ai or, Lithium-sulfur batteries, promise improved properties over LIB. Their research will profit from the 4D imaging capabilities of synchrotron radiation XRD-CT as well. Besides Lithium batteries of any kind, this method can be applied to a vast class of materials, i.e energy materials or other materials and samples that do not absorb x-rays well enough for other methods like SR-µCT.

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