Synchrotron Radiation Nanoscale X-ray Imaging technology and Scientific Big Data Mining Assiste Energy Materials Research

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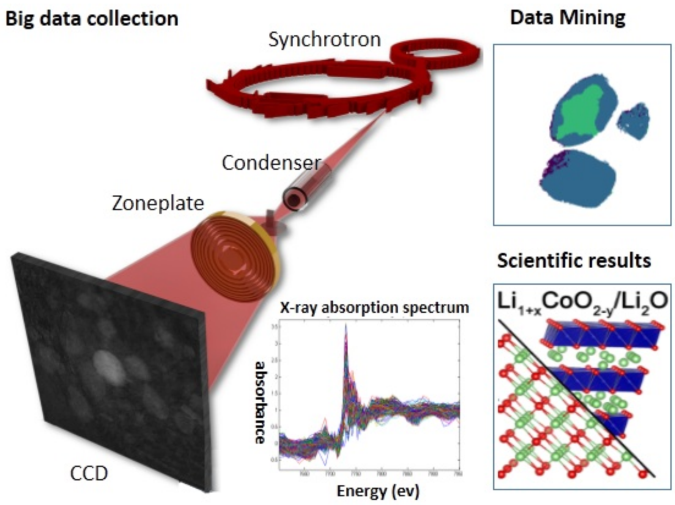
An international research team has applied synchrotron radiation nanoscale x-ray imaging technology and scientific big data mining in an in-situ study of $LiCoO_2$ battery electrodes. The research results can help materials scientists to further improve the properties of battery materials, and are also important for basic scientific research on the failure mechanism of battery materials.

In a paper published earlier this year [ACS Energy Lett. 2, 1240, 2017.], this team demonstrated the in-situ monitoring of a selected LiCoO2 particle over many electrochemical cycles. Their results in that paper suggested that the particle is capable of readjusting itself in response to different local chemical environments. While it is exciting to visualize the individual particle's behavior over long term cycling, scientists will naturally question the representativeness of a single particle to the entire battery cell. To address this question, the team surveyed the battery cell at many different locations. After initial data reduction, they effectively retrieved over 10 million x-ray absorption spectrum covering more than 100 active particles. They developed algorithm for extraction of spectroscopic data attributes, which are then fed into the computing engine for clustering. The developed computing method identified two different particles that are abnormal in terms of their spectroscopic fingerprints. These two particles were further attributed to two different unwanted side reactions that happened during the electrochemical cycling (Figure). This work is recently published in Nano Letters[Nano Lett. 13, 7782, 2017].



Big Data collection: Nanoscale X-ray spectro-microscopy technique (beamline 6-2C of SSRL) collects spatially resolved x-ray absorption spectra at very fast data rate. **Data Mining:** Advanced data mining approach developed in this work searches through over 10 million spectra and identified two particles with unanticipated chemical fingerprints. **Scientific results:** These two particles are attributed to two different unwanted side reactions.