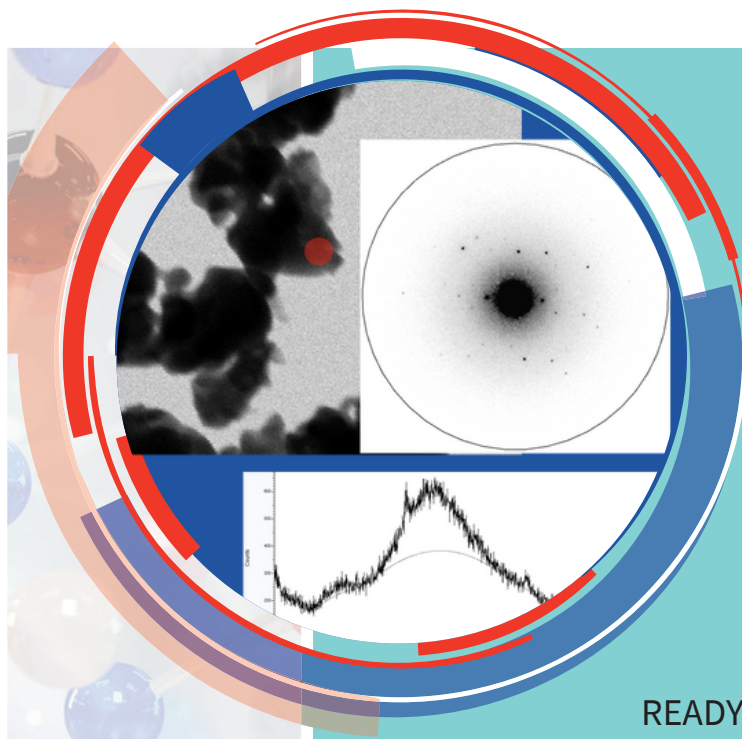


Application Note



Accelerate the Development of Novel Battery Materials using the ELDICO *ED-1* Electron Diffractometer

READY FOR THE FUTURE OF ELECTRON DIFFRACTION

Today 30% of the carbon dioxide emissions are coming from the mobility sector. Within the scope of environmental responsibility, zero carbon dioxide emission batteries for electrical vehicles (EVs) have an important role towards the 'green' energy transition.

For the electrical vehicles industry, the chemistry of batteries plays a crucial role, however, there are certain limitations to overcome. Therefore, exploratory materials and novel battery cell engineering are needed in order to improve the performance in terms of density, range, power, charging times, life span and safety. In this context, solid state batteries (SSB) have gained increased attention. Not only that, but the search for better cathode materials, polyelectrolytes, and the understanding of such systems at the molecular level is key.

In general, the overall performance of such systems is determined by the properties embedded in their atomic structure. To understand the structure-properties relationship, material scientists and engineers need to be able to take a look at the nano-scale levels; the more precisely such structures are understood, the better are the chances to tailor the material properties.

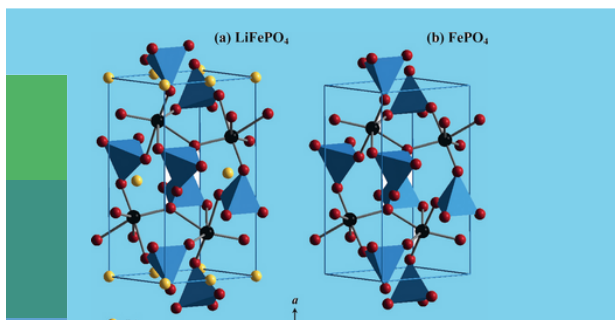
The available analytical methods, such as X-ray diffraction, which provide structural characterization (SC-XRD) have reached their limits. Especially when the materials to be studied are in the nano-scale size.

CHALLENGES

- Limited amounts of materials (few tens of mg)
- Crystals too small for an atomic structure analysis
- Location of light cations (H^+ , Li^+) in combination with heavier metals
- Crystal structures too complex for XRPD

WHAT IS ELECTRON DIFFRACTION?

Electron diffraction combines the best of SC-XRD and XRPD in the battery sector. This allows solid-state chemists and electrochemists, as well as advanced battery developers to obtain precise and accurate structural information of nano-crystalline particles, while providing enough information to even 'see' those light atoms moving within the frame of the heavier atoms.



Crystal structure of $LiFePO_4$ cathode; loaded and unloaded

Applications FOR THE BATTERY SECTOR

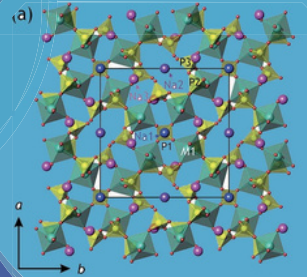
Various states of charges (SOCs) can be structurally characterized

Ab initio structure solution from XRPD is very limited for states of charges. 3D ED can help.

New structures to assist computer modelling for better properties

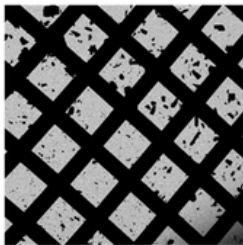
3D ED is of great help as it can give accurate structure determination at the nano scale size levels for materials.

Electron diffraction can be used to solve complex structures not achievable by methods

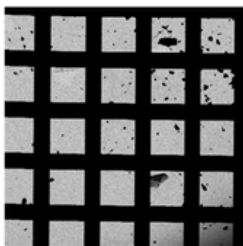


$\text{Na}_7\text{V}_4\text{Al}_x(\text{P}_2\text{O}_7)_4(\text{PO}_4)$

Electron diffraction

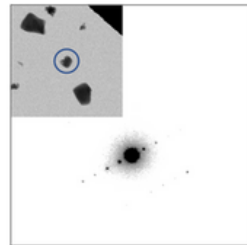


Electron diffraction mapping

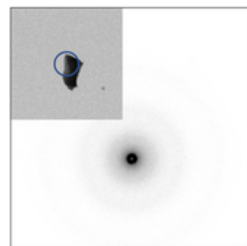


Electron diffraction mapping

Result



91 measured, 26 crystalline



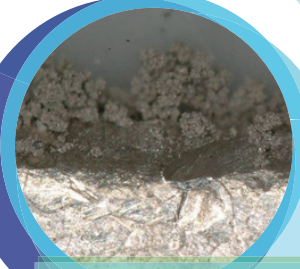
All particles are amorphous

Detection of Crystallinity in Amorphous phases

Electron Diffraction can locally detect crystalline phases in amorphous material which is important to understand the performance of your battery material.

Characterisation of lithium plating through electron diffraction

Given the different crystal structure, lithium dendrites can easily be distinguished from their surroundings.



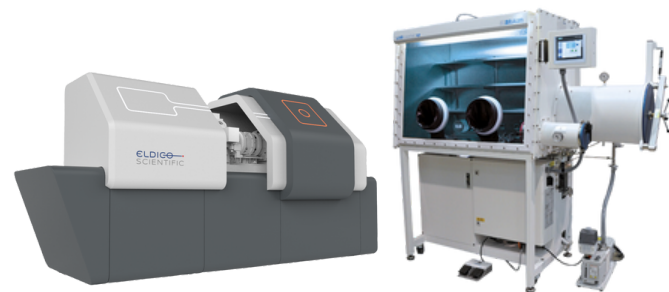
Lithium dendrites

Electron diffraction provides rapid characterisation of amorphicity

Electron diffraction by ELDICO: set-up made for advanced batteries research

ELDICO's Electron Diffractometer, the ELDICO ED-1, is a breakthrough analytical instrument for electron crystallography, enabling investigation of nano-crystalline samples with particle size from 10 to 1000 nm.

ELDICO has a glovebox inhouse to prepare and transfer battery material under an inert atmosphere. The unique design of the ELDICO ED-1 enables to perform automatic phase identification on battery materials.



ELDICO ED-1 with glove box for inert transfer of samples to measurement chamber



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