

# T40. X-Ray Powder Diffraction (XRD) - CERTH



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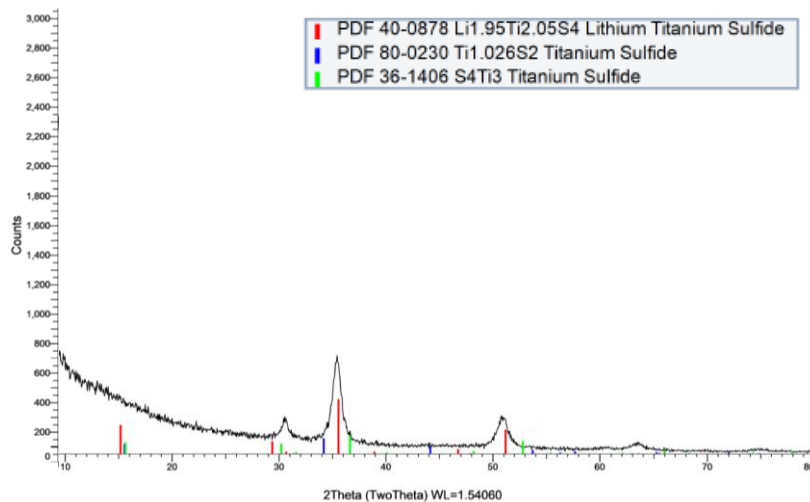
Open Innovation Test Bed for Electrochemical Energy Storage Materials

## How it works

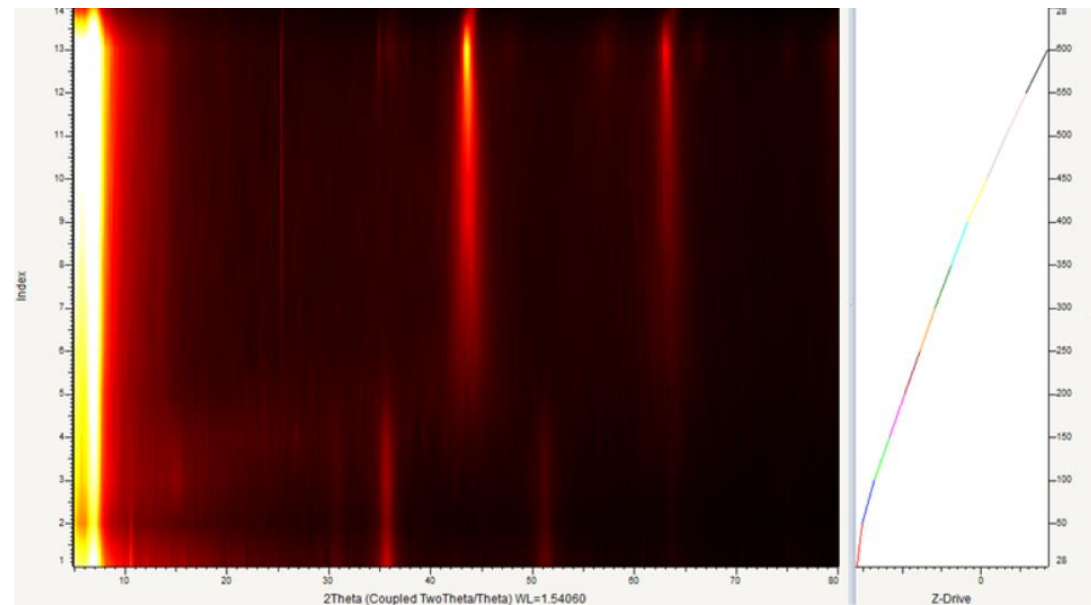
X-ray powder diffraction (XRD) is a rapid analytical technique used for phase identification of crystalline materials and can provide information on unit cell dimensions. X-rays are generated in a cathode ray tube to produce electrons, accelerating them towards a target. When electrons have sufficient energy to dislodge the inner shell electrons of the target material, characteristic X-ray spectra are produced. A detector records and processes this X-ray signal converting it to a count rate.

## What can be seen: Two modes of analysis are possible - examples

- Simple-classic XRD diffractogram (synthesized LTS sample)
- Phase evolution upon heating under a controlled atmosphere by stacking the in-situ individual diffraction patterns at various temperatures



XRD pattern of a synthesized Lithium Titanium Sulfide (LTS) powder



XRD analysis acquired from multiple diffraction patterns showing the evolution of phases (LTS to  $\text{LiTiO}_2$  transition) as a function of temperature under inert (i.e. Ar) atmosphere



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### What kind of sample ?

Typically in powder form or a form that can be processed to produce a powdered material. The analyzed material is finely ground, homogenized and average bulk composition is determined by the analysis.

### Why is it useful ?

XRD is useful for identifying the composition of crystal structured inorganic materials, including the ones used for the batteries key components. Ex-situ analysis and analysis under controlled atmosphere/temperature are performed to generate information on materials structural stability and definition of transitions involved upon their exposure to different conditions.

**Investigation time-scale:** few days to couple of weeks depending on the type of request & form of provided sample

**Maturity level:** advanced

