POLiS
Post Lithium Storage
Cluster of Excellence

STOE STADI P Powder X-ray Diffractometer

Description

Powder X-ray Diffraction (XRD) is an analytical technique used to determine the crystal structure, phase composition, and other structural properties of powdered materials by measuring the diffraction patterns of X-rays interacting with the sample.

- Identifies crystalline phases in electrode materials.
- Monitors structural changes during battery charge/discharge cycles.
- Determines purity and crystallinity of synthesized materials.

Specifications

The STOE STADI P, a high-precision two-circle goniometer, is the foundation of STOE's modular powder diffraction system. It is horizontally mounted and designed in a Transmission/Debye-Scherrer geometry.

- Pure Kα1 radiation using Mo and Ag sources with 0-140^0 2θ range.
- Transmission holder, capillary, operando-coin cell and lab PDF (pair distribution function). measurements possible with Ag Kα1 data.
- Measurement of multiple samples (15) possible.
- Air/moisture-sensitive sample holder available.
- No height displacement and lesser preferred orientation effects due to Transmission geometry.
- WINX^{pow} software is equipped with profile fitting, indexing and lattice constant refinements, theoretical pattern generation and size/strain analysis.

Case studies

1. Tracking the structural changes in single crystal cathodes for Na-ion battery

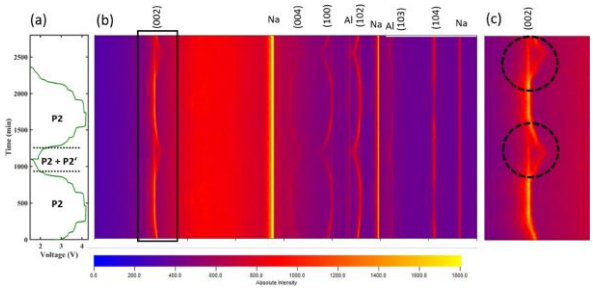

Fig 1:Operando x-ray diffraction data of single crystal P2−$Na_{0.67}Mn_{0.67}Ni_{0.33}O_2$ [1]

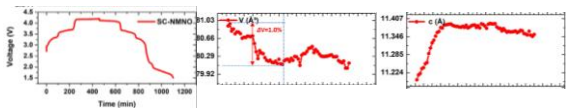

Fig 2:Variation of lattice parameters for first cycle, calculated form operando x-ray diffraction data

2. On the influence of the coherence length on the ionic conductivity in mechanochemically synthesized sodium-conducting halides

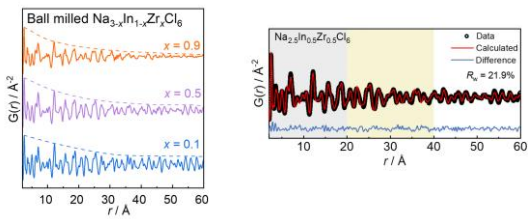

Fig 3:Pair distribution functions of ball milled $Na_{3-x}In_{1-x}Zr_xCl_6$ solid electrolytes measured in a Stoe STADI P (Ag source) [2]

Publications

1) V. Pamidi, C. Naranjo, S. Fuchs, H. S. Stein, P. Barpanda, M. Fichtner,*ACS Appl. Mater. Interfaces* **2024**,*16*, 25953-25965.

2) T. Zhao, A. N. Sobolev, M. A. Craft, C. G. Zeier, *J. Mater. Chem. A.* **2024**, *12*, 7015.