# Driving XRD
# **in Battery Analysis**

XRDynamic 500

# Ensure Optimal
## Battery Performance

Research, development, and utilization of Li-ion batteries is one of the fastest growing industrial segments in the world. Numerous products, including phones, laptops, drones, cars, and now even aircraft, rely on batteries for power. This has led to surging demand for new battery materials and technologies. They may even go beyond Li, with Na or Mg considered promising higher-availability alternatives. Whether with Li-ion or another technology, ensuring batteries are safe, powerful, and reliable is more critical than ever before.

The safety, performance, and lifetime of a battery are linked to the properties of the materials that go into making it, including their crystal structures. Electrodes, separators, current collectors, and all other components need to be fully characterized and monitored throughout the development and manufacturing processes. X-ray diffraction (XRD) plays a crucial role in this characterization as a non-destructive method that delivers detailed structural information at the atomic level. In modern XRD systems, this not only applies to individual battery components measured ex situ but even to complete, functioning batteries via in situ or operando measurements.

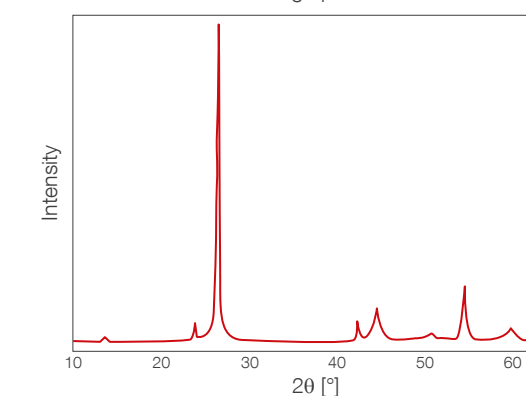**CATHODE (+)**      **SEPARATOR**      **ANODE (-)**

# Optimized for the Demands of
## Battery Research

The outstanding data quality and high degree of automation offered by XRDynamic 500 and the TruBeam™ concept make addressing challenges in battery research easier than ever before. All types of batteries or battery materials can be easily and securely measured on XRDynamic 500, using dedicated sample stages and holders for pouch, prismatic or coin cells, gas-tight sample holders, and much more. Local structure information on amorphous or semi-crystalline materials can even be obtained via PDF analysis.

For the measurement of complete batteries (e.g., coin or pouch cells), the traditional Cu radiation may not be the ideal choice, especially for measurements in transmission geometry. Hard radiation such as Mo or Ag is recommended, and XRDynamic 500 offers suitable X-ray sources and optics for hard radiation setups.

For Mo and Ag radiation, the detector configuration is also critical. Solid-state pixel detectors with CdTe sensors, such as the Pixos 2000 CdTe, offer the highest efficiency for faster measurements in comparison to detectors with Si sensors.


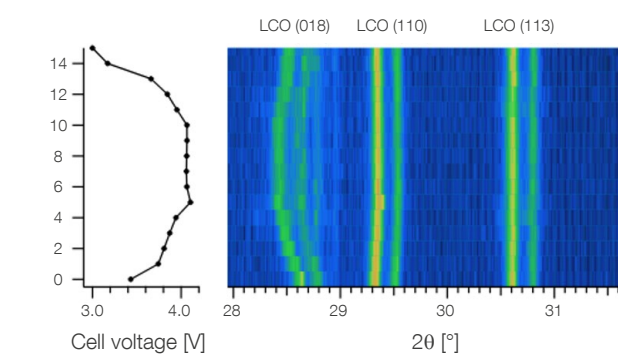XRD measurement of a graphite anode material


Operando XRD measurement of a pouch cell

| Crystallite size [nm] | Degree of graphitization [%] |
| --- | --- |
| 41.2 | 92.7 |

**Ex situ structural characterization of battery materials**

Whether characterizing anode or cathode materials, electrolytes or separators, the structural information obtained from XRD plays a crucial role in the R&D and quality control of all battery materials.

For example, XRD can be used to study graphite anode materials to obtain important information such as the crystallite size and degree of graphitization, which impact the anode performance.

**Operando and in situ analysis**

Complete, functioning batteries can be studied by XRD during the charging or discharging process in so-called in situ or operando measurements when connected to an external potentiostat. This allows structural changes that occur in the different components to be tracked during charge cycling.

For example, in Li-ion batteries, the crystal lattices of the anode and cathode materials swell or contract as Li diffuses from the cathode to the anode and back. This process causes peak shifts in the diffraction patterns, which can be used to gain a deeper understanding of battery stability, degradation mechanisms, or Li diffusion paths.
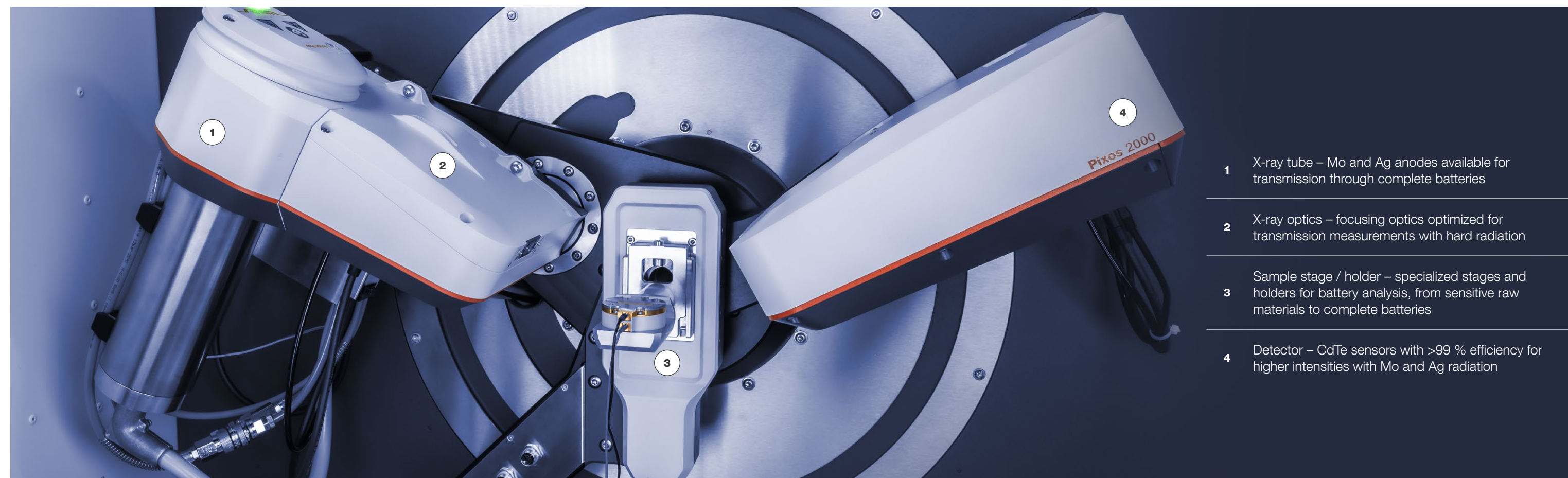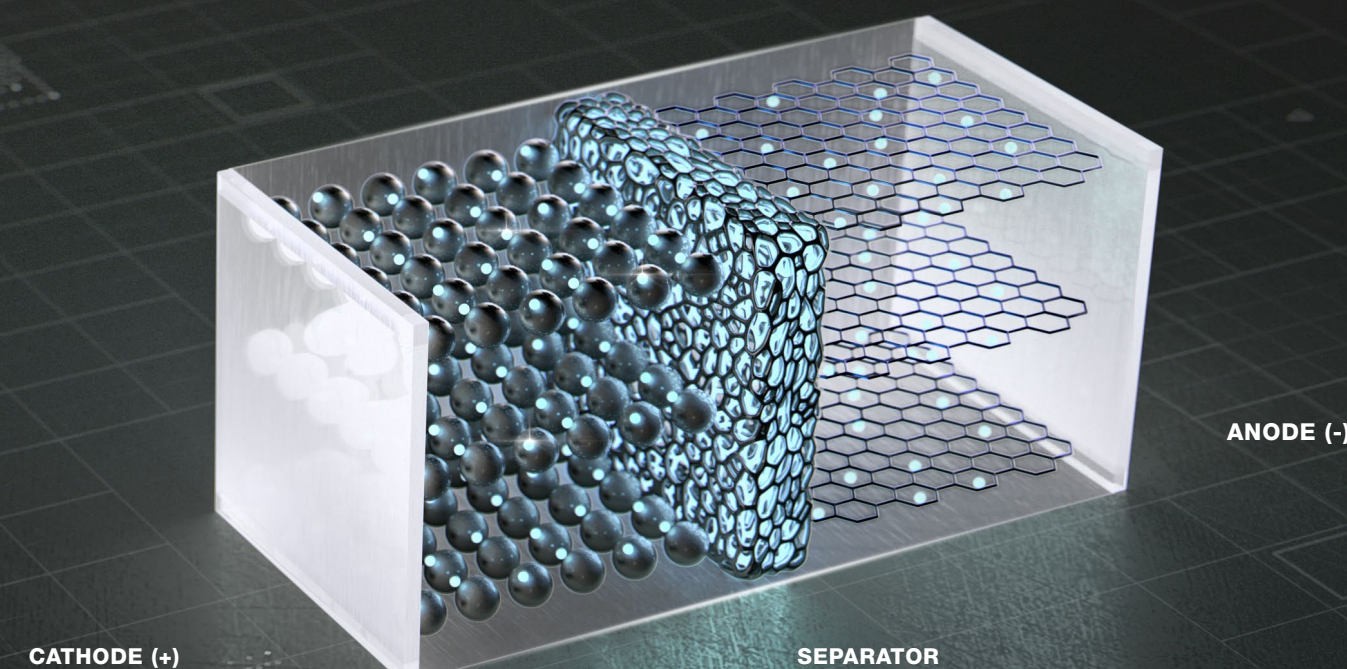


1. X-ray tube – Mo and Ag anodes available for transmission through complete batteries

2. X-ray optics – focusing optics optimized for transmission measurements with hard radiation

3. Sample stage / holder – specialized stages and holders for battery analysis, from sensitive raw materials to complete batteries

4. Detector – CdTe sensors with >99 % efficiency for higher intensities with Mo and Ag radiation

# XRDynamic 500
# Configuration Overview

| | Raw materials | Coin cell (operando) | | Pouch / Prismatic cell (operando) | Electrode (operando) |
| --- | --- | --- | --- | --- | --- |
| | | Ambient | Non-ambient | | |
| **XRDynamic 500 solution** | Various holders, including gas-tight sample holders | Coin cell sample holder | Coin cell holders for TTK 600 | Pouch cell holder | Electrochemical cell |
| **Geometry** | Reflection / transmission | Reflection / transmission | Reflection / transmission | Transmission | Reflection |
| **Recommended radiation** | Cu, Mo | Cu (reflection) Mo, Ag (transmission) | Cu (reflection) Mo, Ag (transmission) | Mo, Ag (transmission) | Cu, Mo |
| **Sample size** | Wide range of diameters and depths | Diameter: 20 mm Thickness: 1.6 mm to 5.5 mm | Diameter: 20 mm Thickness: 1.8 mm | Width: 15 mm to 100 mm Height: 10 mm to 100 mm Thickness: 0 mm to 10 mm | Diameter: Up to 10 mm |

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