Quick guide

Powder X-ray Diffraction (XRD)

In brief

- Analysis of structures and phases in polycrystalline materials
- Qualitative and quantitative phase analysis
- Polymorphic identification and amorphous versus crystalline phase determination
- Crystallite size and preferred orientations
- Thin films analysis: grazing incidence XRD (GIXRD), X-ray reflectometry (XRR)
- In-situ studies: phase transitions and structural investigations

Bold

- **ARL EQUINOX 100 bench-top XRD for routine and research labs**
- **ARL X'TRA Companion bench-top XRD for QA/QC in industrial labs**
- **ARL 9900 XRF-XRD integrated spectrometers for process control**

Applications

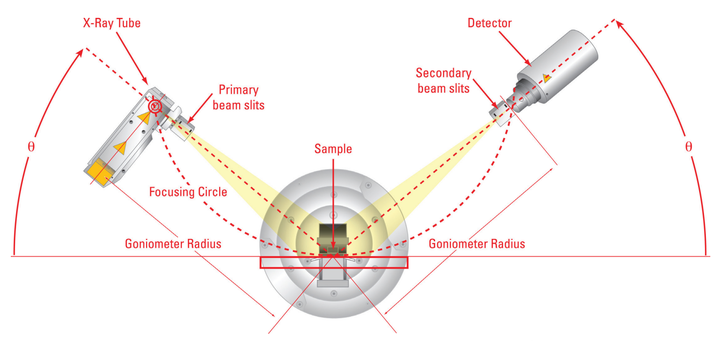
Stand-alone XRD instruments are widely used in both research and industry working on polycrystalline materials:

- Cement and Mining
- Geology and minerals
- Materials science
- Ceramics, metals and other applied materials
- Thin films
- Polymers, catalysts, chemicals
- Energy materials
- Nanomaterials
- Pharmaceuticals
- Semiconductors
- Teaching

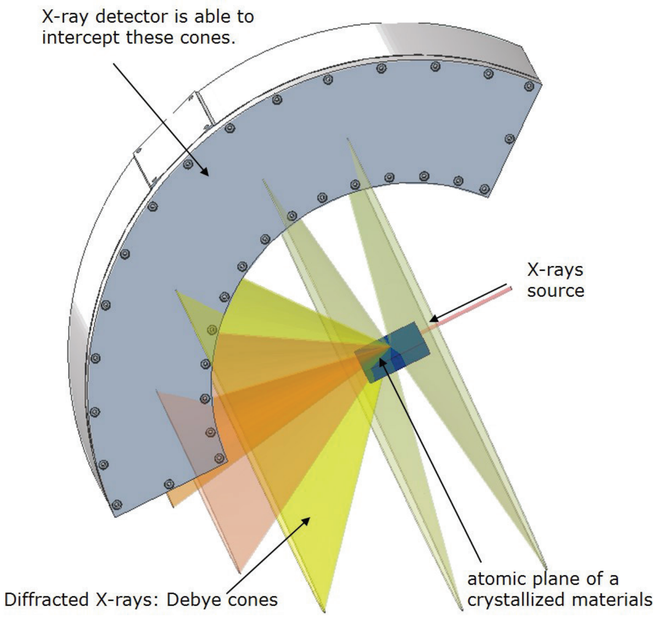
Integrated XRF-XRD instruments also provide a possible analysis solution for routine process and quality control in cement, metals and mining industries.

Basic theory

In X-ray diffraction (XRD) the intensity of X-rays diffracted by the sample are measured according to the diffraction angle (Bragg's law: $\lambda = 2d \sin\theta$, with λ: wavelength, d: d spacing, θ: diffraction angle). Many different diffraction geometries in transmission and reflection exist for powder samples, and the Theta-Theta Bragg-Brentano is the most common one. In contrast to this Bragg-Brentano geometry it is possible to obtain a real-time full pattern without moving parts by using a Thermo Scientific PSD (Position Sensitive Detector). Schematics of both these geometries are shown here. An XRD pattern enables one to do several kinds of analyses like finger- printing of the content by comparing the reflection positions and their relative intensities with the ones from databases. This technique is commonly used for phase control in all kinds of industrial processes.



Bragg-Brentano geometry : ARL X'TRA Companion diffractometer / ARL 9900 XRF-XRD spectrometer



Asymetric mode with a Position Sensitive Detector for real time XRD acquisition: ARL EQUINOX 100

It is also possible to obtain phase identification and quantification or structural information of the phases by applying Rietveld methods in both industrial and university research applications.

Technology

Powder XRD is one of the most established techniques for identifying and characterizing polycrystalline materials with respect to their crystallography, polymorphic structures, phases and crystallinity changes.

Various attachments are used with our powder X-ray diffractometers for making fast acquisitions thanks to fast detectors and for measuring thesample under different forms and environments to study high or low temperature phase transitions, to define thin film characteristics and other properties.

Find out more at **www.thermofisher.com/xrdacademy**

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