

Analysis

Understanding Materials with XRD

X-ray diffraction, or XRD for short, is an analytical method used to study crystalline materials. In this process, the sample is irradiated with X-rays, which are diffracted by the regularly arranged lattice planes of the crystal structure. Based on the measured a characteristic diffractogram is produced from the measured diffraction angles and intensities. This allows conclusions to be drawn about the crystalline phases present, the crystal structure, and other material properties.

What can be analyzed?

Powders, particles, compact specimens, or coated substrates

Phase Analysis: Identification of crystalline phases in samples

Quantitative phase analysis: Determination of phase fractions in mixtures

Crystal structure determination: Analysis of lattice structure and crystal systems

Determination of lattice parameters: Detection of structural changes or doping

Degree of crystallinity: Distinction between amorphous and crystalline components

Particle size estimation: Determination of very small crystallite sizes via peak broadening

Textural analysis: Determination of preferred crystal orientations

Thin-film analysis: Investigation of film thickness, orientation, and quality

In-situ measurements: Investigation of structural changes directly during a process, e.g., during heating, under pressure, or during chemical reactions

Typical fields of application

Catalysts: Identification of active phases and tracking structural changes during a reaction

Battery materials: Analyze existing phases and structural changes in electrode materials

Hydrogen technologies: Evaluate the stability of materials under the influence of hydrogen

Material Development: Characterizing new materials, alloys, or ceramics

Recycling: Characterize residues, slag, ash, or secondary raw materials in terms of their composition

Quality Control: Verifying the Desired Material Composition and Identifying Deviations

Geology and Mineralogy: Identification of mineral phases in rocks, soils, and ores

Measurement Conditions and Equipment Options

- Use of various X-ray sources (Cu, Mo)
- Measurements in reflection and transmission geometries
- Measurements with small sample quantities
- In-situ measurements under realistic conditions
- Use of various gases (H₂, N₂, air etc.)
- Analyses at temperatures up to 900 °C and pressures up to 10 bar(g)
- Flexible bed configurations, such as flow around or through the sample

Benefits for Research and Industry

- Gain a better understanding of materials and develop them in a targeted manner
- Track processes under realistic conditions
- Reliably evaluate the quality and stability of materials
- Identify sources of error and undesirable phases at an early stage
- Experiments can be planned more effectively and development costs can be reduced.

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