# *Test Report on Phase Analysis of Bauxite Using the AMI Lattice XRD*

## 1. Background

Bauxite is the primary raw material used in alumina refining and aluminum smelting, and its mineralogical composition directly influences digestion efficiency, energy consumption, and final product quality. Aluminum-bearing phases such as gibbsite, together with iron-containing minerals including goethite and hematite, determine the reactivity of the ore during processing and the formation of residues. Accurate identification and quantification of these crystalline phases are therefore essential for optimizing mineral processing routes, selecting appropriate smelting technologies, and ensuring raw-material quality control.[1]

Conventional chemical analysis methods can determine total elemental composition but cannot distinguish between different crystalline phases or polymorphs that share similar chemistry. X-ray diffraction (XRD), when combined with Rietveld refinement, overcomes this limitation by using unique diffraction fingerprints to enable rapid and quantitative phase analysis in complex multiphase materials. This approach is widely adopted in the aluminum industry for assessing bauxite quality and verifying compliance with international standards.[2,3]

In this application note, bauxite standard reference material GBW(E)070169 was analyzed using the **AMI Lattice X-Ray Diffractometer.** The objective was to verify instrument performance and demonstrate reliable qualitative and quantitative phase analysis in accordance with international testing standards. θ/θ continuous scanning and full-pattern Rietveld refinement were employed to identify the mineral phases present and determine their relative contents with high accuracy.

## 2. Experiment

The tested sample was the bauxite standard reference material GBW(E)070169, certified for homogeneity and traceability and commonly used for validating XRD phase-analysis methods. Sample preparation followed ASTM E1915-20 guidelines to minimize preferred orientation and peak broadening effects.[4] The material was moderately ground to achieve uniform particle size and then sieved through a 300-mesh screen to remove coarse particles. The resulting powder was loaded into an aluminum sample holder and gently flattened with a glass plate to produce a smooth, gap-free surface suitable for diffraction measurements.

| Parameter | Value |
|---|---|
| Radiation Source | Cu Kα(λ=0.15406 nm) |
| Tube Voltage/Current | 40 kV/20 mA |
| Scanning Mode | θ/θ Continuous Scanning |
| Divergence Slit | 0.2 mm |
| Step Size/Scanning Speed | 0.018°, 3°/minute |
| Scanning Angle Range | 10°-80° (2θ) |

*Table 1: XRD experiment parameters*

All measurements were performed using the **AMI Lattice X-Ray Diffractometer**, and the parameters are described in Table 1.

The analysis strictly followed international standards, including ISO 19950:2015 and ASTM D4926-20, to ensure result comparability and technical credibility.[5,6] Qualitative phase identification was performed by matching measured diffraction peaks with entries in the ICDD Powder Diffraction File database. Quantitative analysis was carried out using Rietveld refinement, with data quality assessed against established signal-to-noise and fitting criteria.(7)

## 3. Results

### 3.1 Qualitative Phase Identification

The XRD pattern of the standard reference material, shown in Figure 1, exhibits sharp and symmetrical diffraction peaks, indicating a high degree of crystallinity. Phase identification revealed the presence of three main mineral components. Gibbsite ($Al(OH)_3$) was identified as the dominant phase, with characteristic reflections at 2θ = 18.2°, 20.2°, and 37.6°, consistent with PDF #97-000-6162. Goethite (FeO(OH)) was identified by reflections at 2θ = 21.2°, 33.2°, and 36.7°, matching PDF #97-024-5057. Minor amounts of hematite ($Fe_2O_3$) were detected through reflections at 2θ = 24.1° and 35.6°, corresponding to PDF #97-008-2135. No quartz or kaolinite was observed, in agreement with the certified composition of the reference material.

Figure 1 presents the measured diffraction pattern together with the Rietveld-refined fit, demonstrating excellent agreement between experimental and calculated profiles.

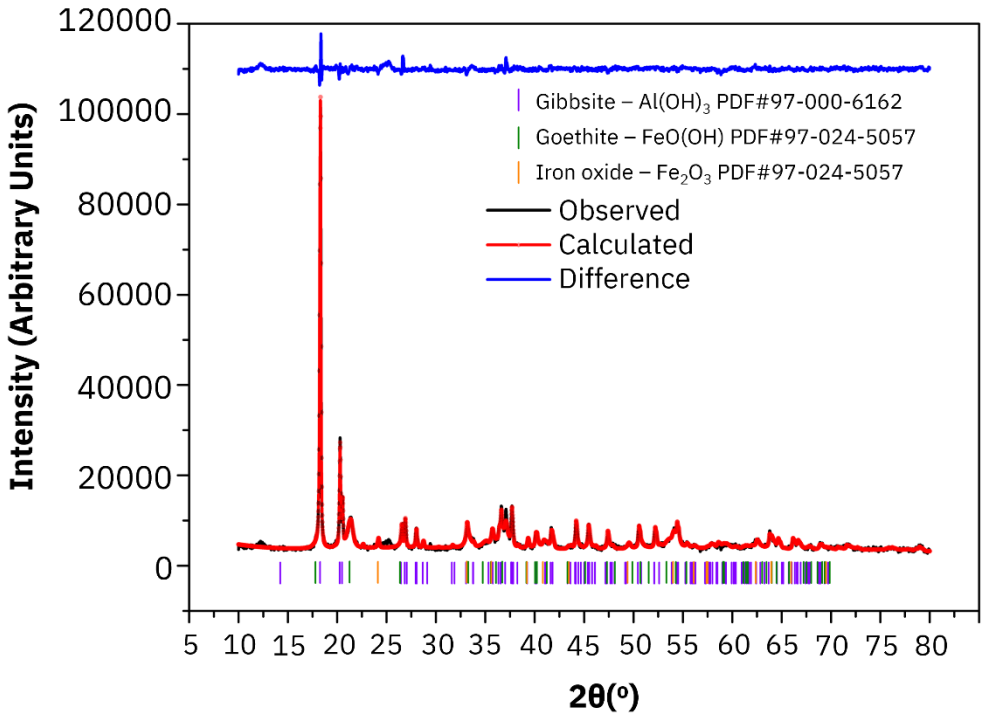


*Figure 1: XRD pattern and structural refinement of bauxite standard reference material GBW(E)070169*

### 3.2 Quantitative Phase Analysis

Quantitative phase analysis was performed using whole-pattern fitting based on Rietveld refinement. The calculated diffraction pattern closely matched the experimental data, indicating a high-quality refinement and reliable phase quantification. The results, summarized in Figure 2a, show that the sample contains 73.9% gibbsite ($Al(OH)_3$), 22.2% goethite (FeO(OH)), and 3.9% hematite ($Fe_2O_3$) by mass.

Refined crystal structures and unit-cell parameters were also determined for each phase. Gibbsite was identified as monoclinic with space group $P2_1/n$ and cell parameters a = 8.66635 Å, b = 5.06966 Å, c = 9.71814 Å, and β = 94.514°. Goethite exhibited an orthorhombic structure with space group Pbnm and cell parameters a = 4.58279 Å, b = 9.96430 Å, and c = 2.98772 Å. Hematite was determined to have a hexagonal structure with space group R-3c and cell parameters a = b = 5.02608 Å and c = 13.75534 Å. Schematic representations of these crystal structures are shown in Figures 2b, 2c, and 2d.

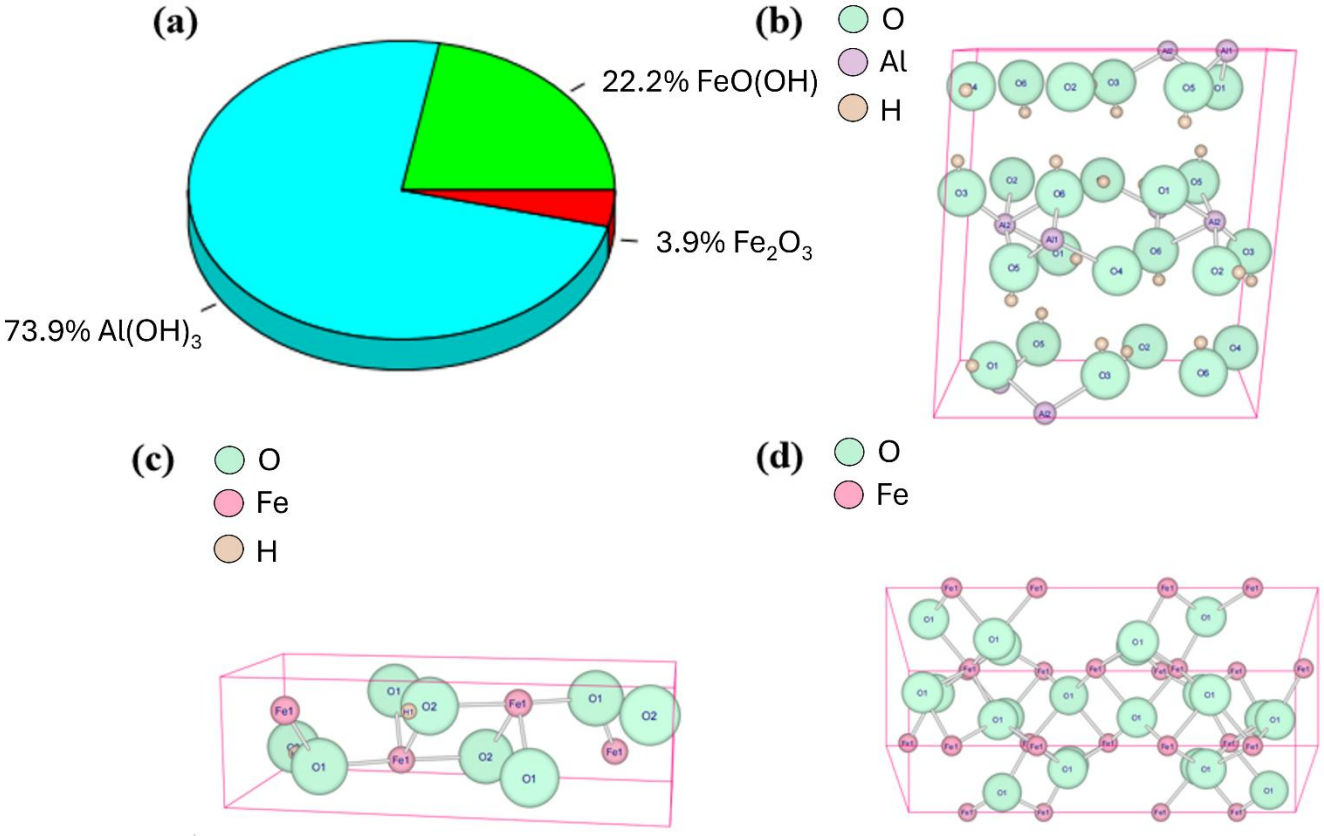


*Figure 2: Bauxite standard reference material GBW(E)070169 a) phase content composition and schematic diagrams of b) gibbsite, c) goethite, and d) hematite*

### 3.3 Instrument Performance Verification

Instrument performance was evaluated using both resolution and efficiency metrics. The full width at half maximum of the main gibbsite peak at 2θ = 18.2° was measured at 0.155°, satisfying the resolution requirements specified in ASTM D4926-20.[6] The total scan time was approximately 25 minutes, providing an effective balance between measurement accuracy and throughput for routine industrial analysis.

These results confirm that the **AMI Lattice X-Ray Diffractometer**, shown in Figure 3, delivers the resolution, stability, and efficiency required for reliable phase analysis of bauxite and related mineral materials.

## 4. Conclusions

The **AMI Lattice X-Ray Diffractometer,** combined with Rietveld refinement, successfully performed both qualitative and quantitative phase analysis of the bauxite national standard reference material GBW(E)070169 in full compliance with international standards. The identified phase assemblage and quantified contents closely match the certified values, demonstrating the accuracy and reliability of the measurement approach.

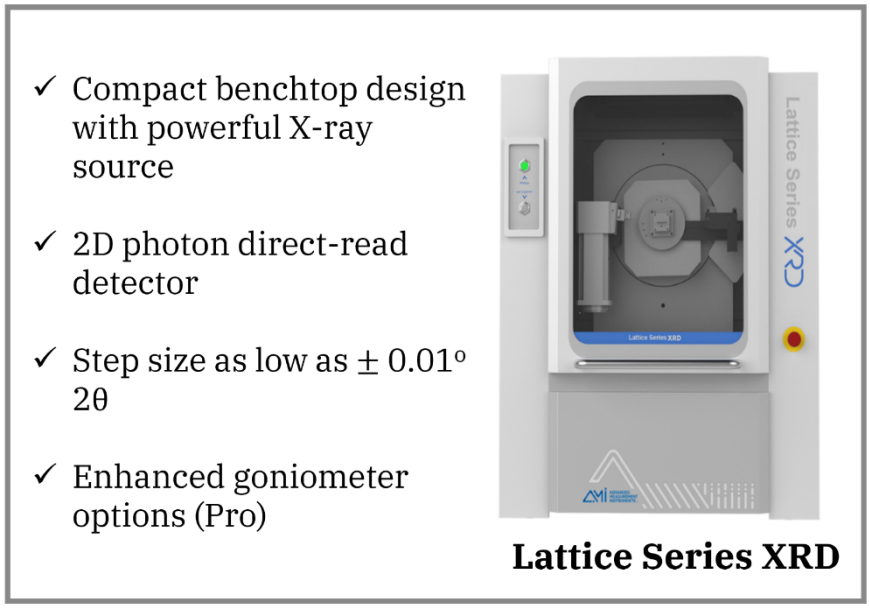


*Figure 3: Highlighted features of the **Lattice Series XRD** from **AMI***

Instrument performance metrics confirm excellent angular resolution, repeatability, and data quality, making the **AMI Lattice XRD** well suited for routine phase analysis in aluminum smelting and mineral processing workflows. The ability to rapidly identify and quantify key mineral phases provides valuable support for raw-material assessment, process optimization, and quality assurance. Raw diffraction data and refinement logs can be provided upon request to facilitate further customer validation or integration into process-development studies.

All standards and references cited in this report were verified against official standards databases and authoritative crystallography literature to ensure technical validity and traceability.

## 5. References

(1) *Smelter Grade Alumina from Bauxite: History, Best Practices, and Future Challenges.* Springer Series in Materials Science, Raahauge, B. E., Williams, F. S. Eds.; Springer Nature, 2022.
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(4) ASTM E1915-20, Standard Test Methods for Analysis of Metal Bearing Ores and Related Materials for Carbon, Sulfur, and Acid-Base Characteristics. ASTM International, 2020.
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