Application note | 41507

X-ray diffraction

Determination of $\mathit{A}\mathrm{AL_2O_3}$ and $\mathit{R}\mathrm{SiO_2}$ in bauxite ores

ARL X'TRA Companion X-Ray Diffraction System

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Introduction

The precise characterization of bauxite ores is essential for optimizing aluminum production processes. X-ray diffraction (XRD) is a powerful analytical technique that provides detailed insights into the mineralogical composition of bauxite ores, particularly focusing on active alumina ($\mathit{A}\mathrm{Al_2O_3}$) and reactive silica ($\mathit{R}\mathrm{SiO_2}$). These two parameters are critical performance criteria in the Bayer process, which is the predominant method for extracting alumina from bauxite.

Active alumina, primarily in the form of gibbsite, boehmite, and diaspore, determines the efficiency and yield of the alumina extraction process. Reactive silica, often present as kaolinite and quartz, can form undesirable sodium aluminosilicate phases during digestion, reducing alumina recovery and increasing operational costs.

The application of XRD in quantifying active alumina and reactive silica in bauxite ores has advantages over traditional wet chemical analysis methods because it provides rapid, non-destructive, and precise mineralogical data. Additionally, eliminating hazardous chemicals from the procss protects the environment and saves cost.

By understanding the mineralogical intricacies of bauxite ores through XRD, industry professionals can enhance process efficiency, reduce impurities, and optimize resource utilization, ultimately leading to more sustainable and cost-effective alumina production.

Instrument & software

The Thermo Scientific™ ARL™ X'TRA Companion XRD System (c.f. Figure 1) is a simple, easy-to-use benchtop XRD instrument for routine phase analysis as well as more advanced applications. The ARL X'TRA Companion XRD System uses a θ/θ goniometer (160 mm radius) in Bragg-Brentano geometry coupled with a 600 W X-ray source (Cu or Co). The radial and axial collimation of the beam is controlled by divergence and Soller slits, while air scattering is reduced by a variable beam knife. An integrated water chiller is available as an option. Thanks to the state-of-the art solid state pixel detector (55 x 55 µm pitch), the ARL X'TRA Companion instrument provides very fast data collection and comes with one-click Rietveld quantification capabilities and automated result transmission to a LIMS (Laboratory Information Management System) seamless integrated into Thermo Scientific™ SolstiX™ Pronto Instrument Control Software.

Figure 1. ARL X'TRA Companion Diffraction System.

Experimental

Bauxite CRMs BCS 395 and NIST 696 were measured in reflection mode using Cu Kα (1.541874 Å) radiation for 10 minutes (5-65° 2θ). Data acquisition was performed with spinning sample and electronic photon energy filtering to reduce sample fluorescence (c.f. Figures 2 and 3). Quantitative analysis (Rietveld method) was performed by Profex software (BGMN) and AAl_2O_3 (boehmite and gibbsite) and $RSiO_2$ (clays and quartz) were calculated.

Results & discussion

Phase identification and quantification show high amounts of alumina and low amounts of silica bearing phases (c.f. Table 1). Certified elemental composition is in good agreement with results calculated from Rietveld refinements. Deviations are most likely due to variations from database composition of constituents which is very likely for natural samples (c.f. Table 2).

This results in AAl_2O_3 54.4 % (BCS 395) and 54.5 % (NIST 696) with $RSiO_2$ 1.0 % (BCS395) and 4.4 % (NIST 696) respectively.

Both samples qualify as high-quality ores to be used in the Bayer process.

Conclusion

Data from the ARL X'TRA Companion Diffractometer System measured in 10 minutes is perfectly suited to determine AAl_2O_3 and $RSiO_2$ in bauxite ore samples due to the high-performance detector and exceptional photon energy filtering. The SolstiX Pronto Software reduces the operator burden by making one-click analysis accessible to everyone and increases your efficiency while still maintaining high quality results.

	Composition (in wt %)	
Phases	**BCS 395**	**NIST 696**
Gibbsite $Al(OH)_3$	80.3	83.4
Boehmite AlO(OH)	1.9	N/A
Hematite Fe_2O_3	5.1	2.0
Goethite FeO(OH)	9.1	4.3
Anatase TiO_2	0.3	1.9
Rutile TiO_2	1.8	0.9
Quartz SiO_2	0.6	1.8
Kaolinite $Al_4Si_4O_{10}(OH)_8$	N/A	5.7
Nacrite $Al_4Si_4O_{10}(OH)_8$	1.0	N/A

Table 1. Refinement results of BCS 395 and NIST 696.

BCS 395 (in wt%)	LOI	Al_2O_3	SiO_2	TiO_2	Fe_2O_3
XRD	28.0	54.8	1.0	2.1	14.1
Certificate	27.8	52.4	1.2	1.9	16.3
BCS 696 (in wt%)	**LOI**	**Al_2O_3**	**SiO_2**	**TiO_2**	**Fe_2O_3**
XRD	29.7	56.8	4.4	2.8	6.3
Certificate	29.9	54.5	3.8	2.6	8.7

Table 2. Calculated vs. certified elemental composition of BCS 395 and NIST 696.

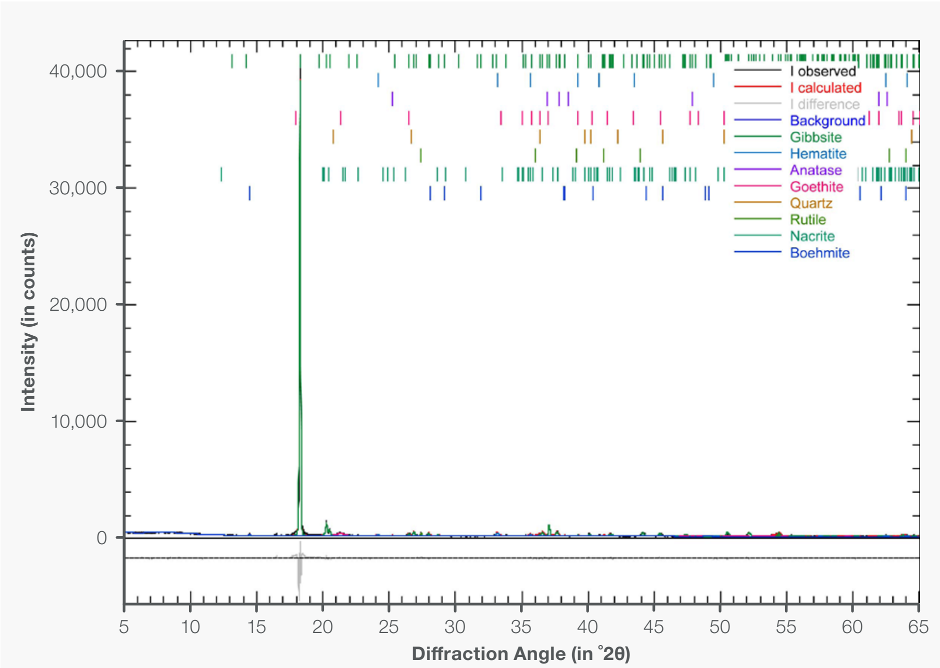

Figure 2. Measurement (10 minutes) of BCS 396 bauxite ore.

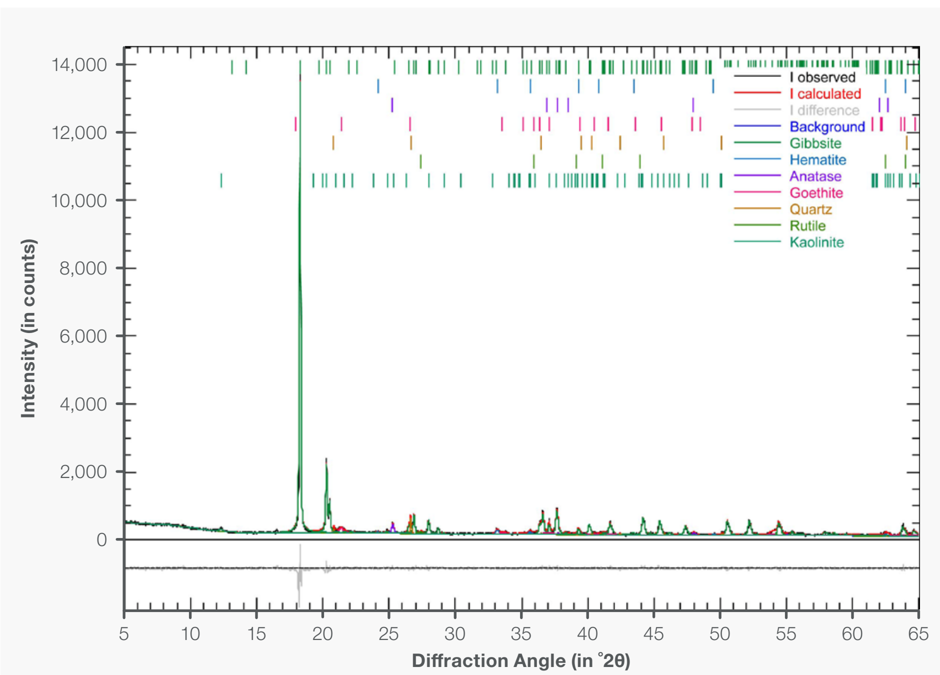

Figure 3. Measurement (10 minutes) of NIST 696 bauxite ore.

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