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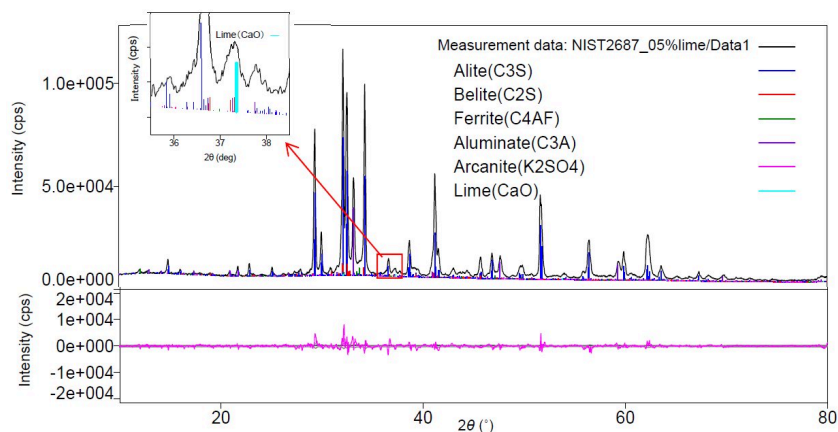
# B-XRD1076 - Rietveld quantitative analysis of trace components In cement

## Introduction

Clinkers, a component of cements, are created by mixing and calcinating limestone, clay and silica sand. The amount of free lime (calcium oxide) is an important factor to confirm the clinker's degree of calcination. When free lime reacts with moisture or carbon dioxide gas in air, the chemical reaction produces calcium hydroxide and calcium carbonate, so a swift measurement is essential to prevent this from happening. In the past, the calibration method was applied to quantitative analysis of cements, but this technique had a difficulty in separating the peaks of free lime since the diffraction peaks of cement components were crowded in the analysis results. In the example below, we used a benchtop X-ray diffractometer mounted with a high-speed 1D detector to achieve swift measurement, and then applied the Rietveld method to perform quantitative analysis on the free lime in cements.

## Measurements and Results

A 10-minute measurement in the range of  $2\theta = 10-80^\circ$  was performed on a simulated sample consisting of NIST2687 standard with 0.5 mass% free lime added. Figure 1 shows the Rietveld analysis result, and Table 1 shows the quantitative analysis result. The Rietveld analysis profile matched well with the observed profile, with a reliability factor ( $R_{wp}$ ) of 5.06%. The amount of free lime also matched the prepared value as well within the range of tolerance. In conclusion, by using a benchtop X-ray diffractometer mounted with a high-speed 1D detector, a high-intensity diffraction profile sufficient to perform a Rietveld quantitative analysis can be collected in a swift measurement, and the content of trace components of 1 mass% or less can be determined with high accuracy.



**Figure 1:** X-ray diffraction profile and Rietveld analysis result.

**Table 1:** Rietveld analysis result

<b>Components</b>	<b>Rietveld quantitative value (mass%)</b>	<b>Adjusted value (mass%)</b>
Alite (C3S)	71.7(3)	71.24±1.27
Belite (C2S)	12.8(3)	12.57±1.22
Ferrite (C4AF)	2.55(8)	2.81±0.68
Aluminate (C3A)	12.19(9)	11.82±1.03
Arcanite (K <sub>2</sub> SO <sub>4</sub> )	0.24(8)	0.92±0.15
Lime (CaO)	0.47(6)	0.52* (Added value)

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