

Sample Holder

D2 PHASER

LYNXEYE

Application Report XRD 11

D2 PHASER Desktop XRD: Quantitative phase analysis of Gypsum/Anhydrite samples

The D2 PHASER is a portable desktop XRD instrument for research and quality control. It is easy to operate and independent of external media such as cooling circuits. Thanks to the LYNXEYE detector it is the fastest desktop XRD system on the market. The system delivers high quality measurement data, which allows performing advanced analytical methods, such as the standardless quantitative Rietveld phase analysis. This report demonstrates its use for the determination of the different sulphate phases in natural Gypsum or Anhydrite.

Tab. 1: Experimental settings.

D2 PHASER, LYNXEYE detector
Cu radiation (30 kV, 10 mA), Ni filter
Continuous scan from 8 to 65° 2Theta Step width 0.02° Counting time 0.5 sec per step
Total scan time about 26 min.
2.5° Soller slits, 1.0 mm divergence slit, anti-scatter screen
LYNXEYE detector opening 5° 2Theta

X-ray powder diffraction combined with TOPAS Rietveld analysis is nowadays one of the most powerful methods existing, to perform quantitative phase analysis. In the last years it became a standard tool in research and development, but also in the minerals and mining industries.

Natural Gypsum is often a mixture of the sulfate phases Gypsum ($\text{CaSO}_4 \times 2\text{H}_2\text{O}$), Hemi-hydrate ($\text{CaSO}_4 \times \frac{1}{2}\text{H}_2\text{O}$) and Anhydrite (CaSO_4). These phases do have different physical properties, e.g. solubility. Elemental analysis is not able to distinguish these minerals, therefore often DSC/TG methods are used. They require calibration efforts and are time consuming. XRD offers a simple and straightforward solution.

A Gypsum sample of natural origin was analyzed, to demonstrate the performance of the D2 PHASER for such applications. The measurement covered the angular range from 8 to 65° 2Theta. The scan time was about 26 minutes. Experimental details are summarized in Table 1. Figure 1 shows the measured data as well as the results of the TOPAS Rietveld analysis.

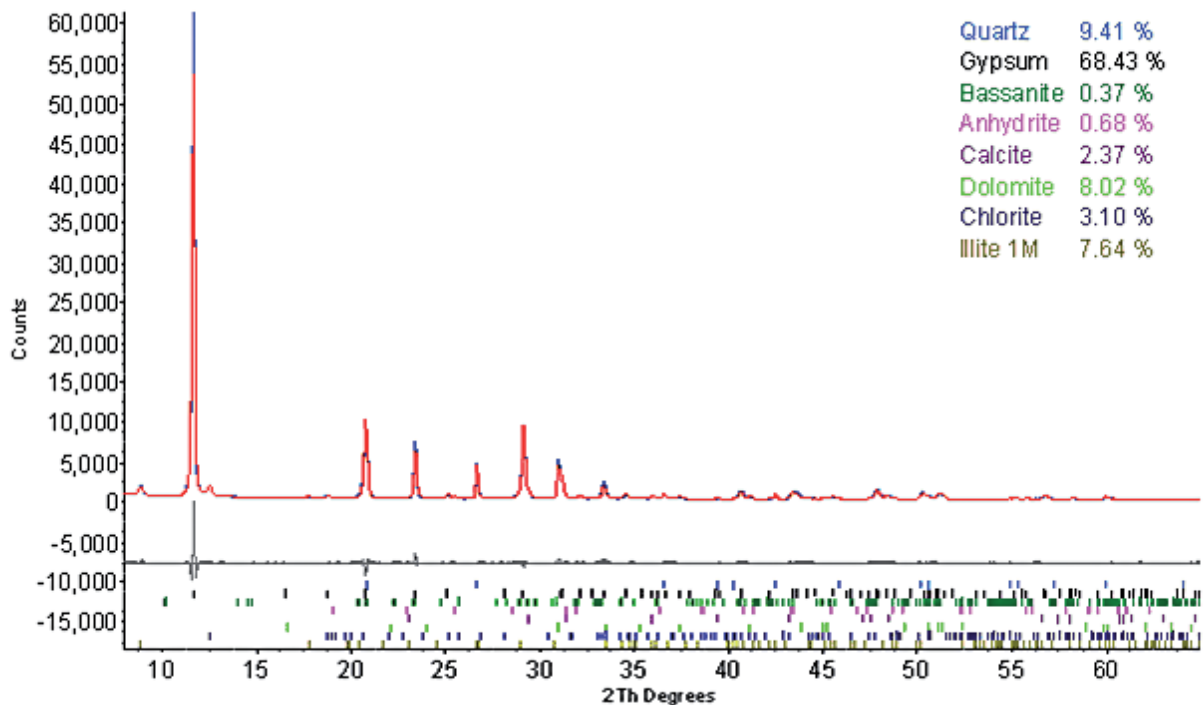


Figure 1: TOPAS Rietveld phase quantification of the Gypsum sample (values given in wt. %). The blue curve is the measured diagram. The red curve is the calculated diagram. In grey the difference of both is given. The marks below indicate the possible peak positions of each phase.

To conclude, our cost-effective desktop XRD system D2 PHASER, equipped with the 1-dimensional LYNXEYE detector, provides high quality data, which allows doing accurate quantitative phase analysis of the sulphate phases Gypsum, Hemi-hydrate and Anhydrite in natural rocks and flue gas purification products.

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