Application note

Decarbonized cements and the benefits of XRD analysis

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Introduction

Due to the ongoing climate crisis, there is a strong requirement to increase the energy efficiency of advanced material production processes. The production of classical cement is responsible for about 8% of global CO_2 emissions, and clinker production accounts for most of these emissions. Therefore, new technologies are being developed to reduce the carbon footprint of cement-like materials.

There are different approaches in the development of decarbonized cement-like materials:

1. Reduce the amount of clinker required
2. Replace clinker with carbon neutral materials
3. Capture the CO_2 required for the process

In each of these approaches, thorough scientific analysis is required throughout development and production. X-ray diffraction (XRD) is a powerful analytical technique to identify crystalline components and quantify them together with potential amorphous content. Advanced analytical software offers options for a standardless approach to quantify the amorphous part of a mixture, which plays a significant role in advanced cement-like materials.

Instrument

The Thermo Scientific™ ARL™ EQUINOX XRD Series represent a portfolio of XRD instruments ranging from simple, easy-to-use benchtop systems for routine analysis to more advanced floor-standing, research-grade systems.

The Thermo Scientific ARL EQUINOX 100 X-ray Diffractometer employs a custom-designed 50 W (Cu or Mo) or 15 W Co high-brilliance micro-focus tube with mirror optics that does not require an external water chiller. The unit can be transported between laboratories or into the field without requiring any special infrastructure.

The ARL EQUINOX 100 Diffractometer provides faster data collection compared to other diffractometers due to its unique curved position-sensitive detector (CPS) that measures all diffraction peaks simultaneously and in real time.

Figure 1. ARL EQUINOX 100 X-ray Diffractometer.

Experimental

Powdered (ball milled) samples were measured in reflection mode using an ARL EQUINOX 100 Diffractometer with Cu Kα radiation. Data evaluation (qualitative and quantitative) was performed using MDI JADE 2010 and ICDD PDF4+ database. Quantification was carried out using WPF Rietveld refinements. A standardless approach for quantification of amorphous content (using pseudo-RiR values) was used.

Results

A novel approach for reducing the clinker content in cement uses a mixture of calcined clay and limestone together with gypsum and clinker. A sample of such a mixture was investigated (Figure 2), consisting of 91% amorphous material (calcined clay), 6% calcite ($CaCO_3$) and 3% natrite (Na_2CO_3).

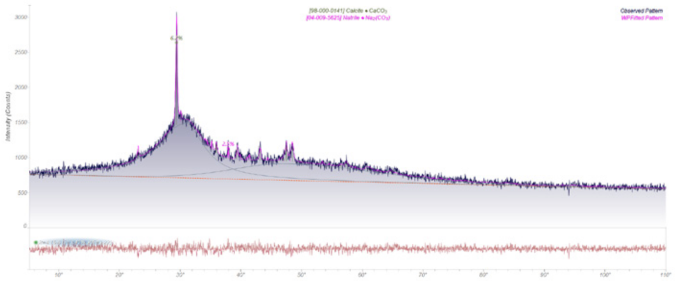

Figure 2. XRD pattern of calcined clay and calcite sample.

Figure 3 shows natural gypsum with a small quartz side phase.

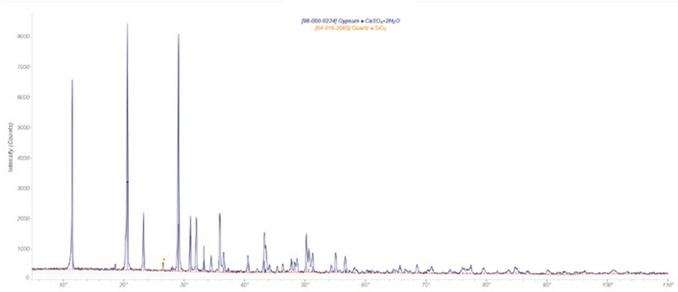

Figure 3. XRD pattern of gypsum sample.

Fly ash (Figure 4), which is an industrial waste product, can be used as a cement-like material to completely replace clinker. Its quality strongly depends on the amorphousness of the material. The fly ash shown in Figure 4 is nearly 100% amorphous with a slight quartz side phase.

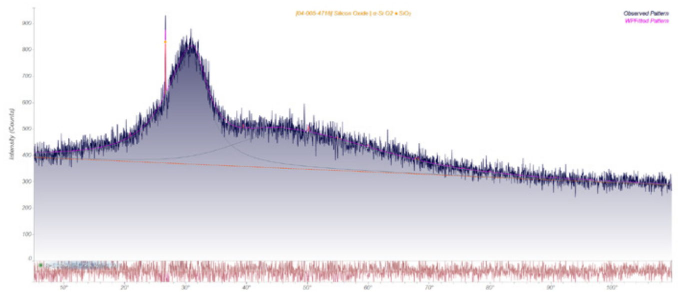

Figure 4. XRD pattern of fly ash sample.

Portlandite (Figure 5) can be added to the cement mixture and afterwards cured with waste CO_2, which dramatically reduces the carbon footprint. A portlandite sample consisting of 39% amorphous material, 51% portlandite, 5% calcite, 4% grossite, and 1% quartz is shown in Figure 5.

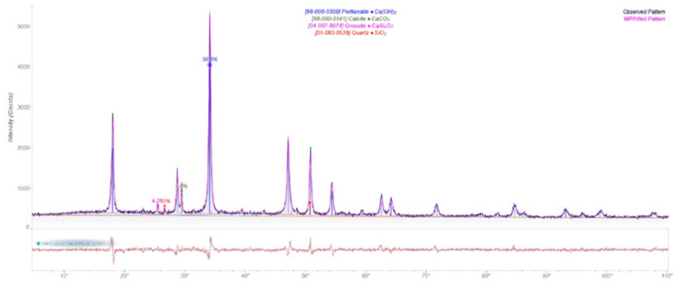

Figure 5. XRD pattern of portlandite sample.

Conclusion

The ARL EQUINOX 100 X-ray Diffractometer produces data perfectly suited for analyzing decarbonized cement-like material samples. Quantifying the amorphous content using a standardless approach has proven to be a powerful technique that directly yields the composition of even complex mixtures.

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