

Thermo Scientific ARL X'TRA Companion

Next-level routine control benchtop
X-ray diffractometer



Introduction

The microstructure of a material reveals connections between its formation process and its final properties. However, the complex and heterogenous qualities of mineral compounds presents constant challenges when studying their microstructures.

For example, the varied compositions of cement or clinker can be adjusted to affect specific properties such as reactivity, setting time, or color. It is well known that reactivity will depend on the C3S/C2S ration, while C3A will influence the setting time, and C4AF will impart a different color to the cement. The quality of products is therefore dependent on the phase minerology of cements.

To ensure a product's desired qualities, accurate and reproducible analyses must be performed. A combination of XRF and XRD appears to be an excellent solution to this challenge, as it is able to provide routine, on-line process and quality control of the various mineral phases.

ARL™ X'TRA Companion

As demand for advanced technology increases, instrumentation keeps pace by advancing in sophistication and performance. However, this does not mean that advanced technology must be synonymous with increased complexity.

The Thermo Scientific™ ARL™ X'TRA Companion has been developed under the premise that high performance and precision should be associated with ease of use and efficiency, for daily operation with complete peace of mind.



ARL X'TRA Companion is a θ/θ Bragg-Brentano benchtop X-ray diffractometer perfectly suited for routine control. Its state-of-the-art configuration uses advanced technical features to deliver accuracy, precision, safety, and ease of use. As a plus, it comes with a one-click data treatment software to ensure reliable results.

Innovative, easy to use XRD benchtop equipment you can rely upon for precision, performance and flexibility

Completely safe

ARL X'TRA Companion components are mounted in a shielded cabinet in accordance with international X-ray safety rules, equipped with lead glass windows, flushing lamps and safety interlocks.

Robust design

ARL X'TRA Companion's sturdy design counteracts disturbances from shock or vibration, allowing it to be deployed in almost any environment.

Enhanced performance

ARL X'TRA Companion θ/θ goniometer is ultra-compact, adopting stepper motors with optical encoders, to ensure extremely precise angular positioning and reproducibility.

High quality data

ARL X'TRA Companion incorporates the latest generation of detector, offering speed and accuracy with superior data quality.

Customizable to your needs

ARL X'TRA Companion provides various dedicated solutions for all types of pressed samples (Polysius, Hertzog, other pressed pellets). These fully meet analytical requirements and optimize data quality.

Intuitive software analysis

ARL X'TRA Companion reveals the full potential of your data thanks to a reliable and easy-to-use analysis software designed to quickly and simply extract the information you are looking for.

Combinable with other data

ARL X'TRA Companion data may be easily combined with XRF data to increase accuracy and allow for more insightful interpretation of results.

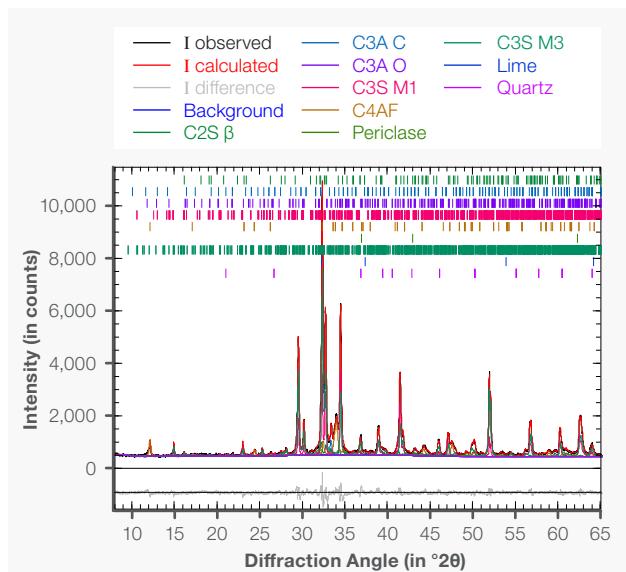
Analysis of Cement Clinker according to ASTM C1365

A clinker sample was measured (21 x 10 min) and a Rietveld fit was carried out consecutively using a fundamental parameter approach. Comparing standard deviations calculated from the repetitive refinements with limits given by ASTM C1365 clearly shows that results are in good agreement with the norm, as determined by considering C3A total and C3S total.

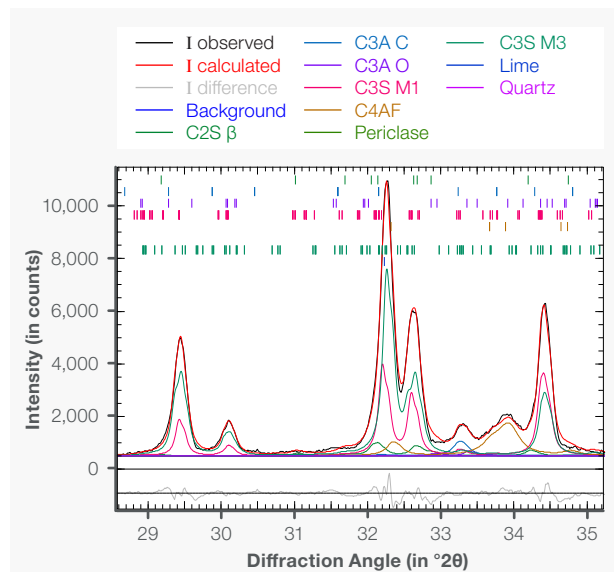
The ARL X'TRA Companion XRD yields data in compliance with ASTM C1365 norm for analyzing clinker samples. The one-click Rietveld refinement based on a fundamental parameter approach is an extremely robust method with high reproducibility which yields accurate results even for C3S M1 and M3. This makes clear the **ARL X'TRA Companion is the perfect solution for any process control tasks in the cement industry.**

	Average values	STDEV	ASTM
	(in %)	(1 σ in %)	C150
C3S M1	30.81	1.08	
C3S M3	46.32	1.08	
C3S Total	77.13	0.25	0.74
C4AF	12.08	0.20	0.64
C2S β	6.09	0.18	0.49
C3A Cubic	2.57	0.34	
C3A Ortho	1.23	0.39	
C3A Total	3.80	0.14	0.47
Lime	0.21	0.06	
Periclase	0.59	0.06	0.23
Quartz	0.10	0.03	

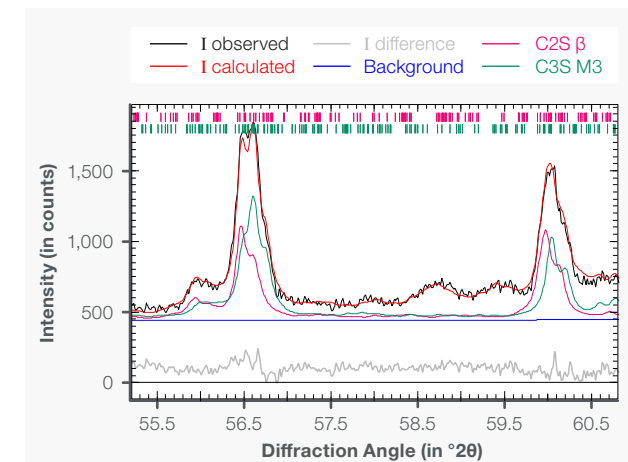
Results of the 21 consecutive refinements of clinker (values in weight percent).



Rietveld fit of clinker (10 min acquisition).



Rietveld fit of clinker (29-35° 2θ).



Measurement of clinker (55-61° 2θ). Fit for C3S M1 (purple) and C3S M3 (green) explains intensity and shape of the reflections well.

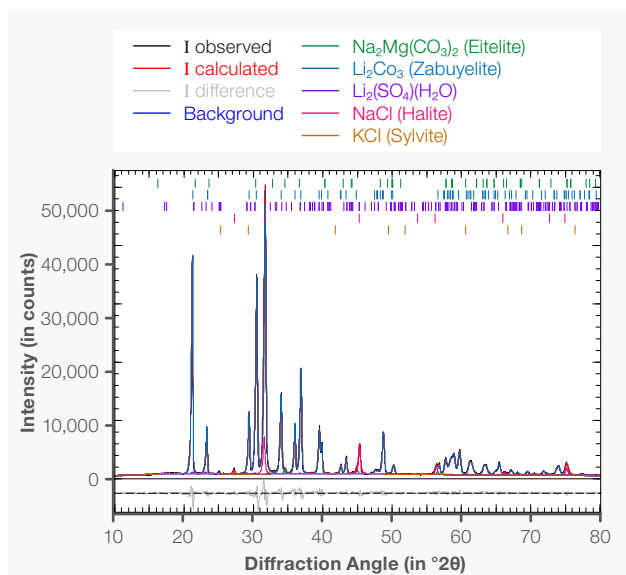
Quality Control of Li_2CO_3 from Salars by XRD analysis

Salars are salt flats or salt pans where lithium is extracted as Li_2CO_3 or LiOH from brines or saltwater through a series of evaporation steps. Lithium carbonate is a widely used material in the production of batteries, ceramics, and glass, among other materials. Its purity and crystallinity are crucial to ensure the quality of the final product. Thanks to the XRD technique, it is possible to control this quality. Two powdered samples of Li_2CO_3 from Salars were measured using reflection geometry. The samples were measured for 10 minutes each. Phase quantification was performed with a one-click Rietveld refinement using a fundamental parameter approach.

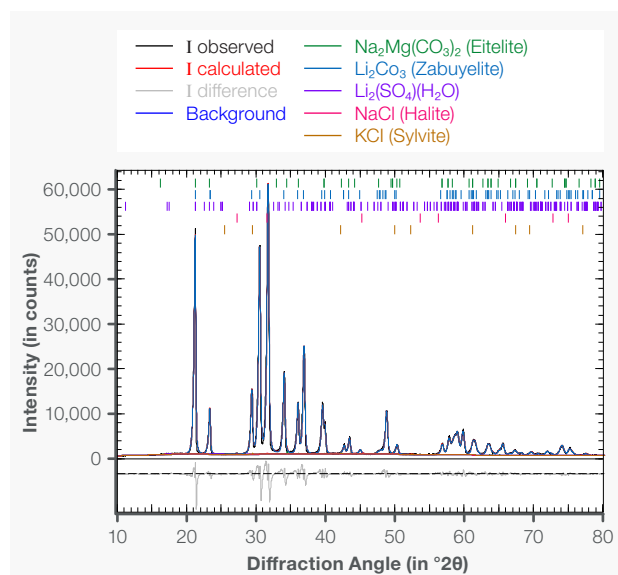
The table shows results from the refinements and allows one to observe that both samples are of different quality. For further processing it is important to have phase-pure material with high total Li content. The Li content can be indirectly ascertained from Rietveld refinements assuming stoichiometric phases with known Li content. Sample A is contaminated with 3.3 wt% NaCl and other minor phases which results in a total Li amount of 18.0 wt%, which is in good agreement with the reference value of 17.2 wt% from chemical analysis. Sample B is of better quality and contains minor contaminations which results in a total Li of 18.7 wt% (reference: 18.5 wt%). Both samples are completely crystalline.

This demonstrates that XRD is a powerful technique to assess the quality and purity of Li_2CO_3 in a short time because it can indirectly measure the total Li content of the sample as well as contaminants which could impact the price and further processing of the material.

In conclusion, the one-click Rietveld refinement based on a fundamental parameter approach is an extremely robust method with high reproducibility and therefore **the ARL X'TRA Companion is the perfect solution for any process control or quality control task.**



Rietveld fit of Li_2CO_3 sample A (10 minutes).



Rietveld fit of Li_2CO_3 sample B (10 minutes).

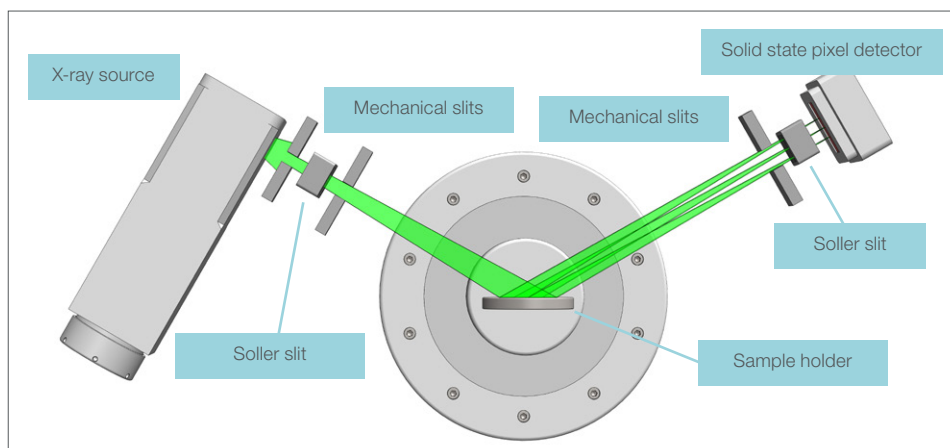
Phase	Sample A (in wt%)	Sample B (in wt%)
$\text{Na}_2\text{Mg}(\text{CO}_3)_2$ (Eitelite)	0.7 (1)	0.2 (1)
Li_2CO_3 (Zabuyelite)	95.3 (2)	99.5 (2)
$\text{Li}_2(\text{SO}_4)(\text{H}_2\text{O})$	0.7(1)	0.2 (1)
NaCl (Halite)	3.3 (1)	0.1 (1)
KCl (Sylvite)	0	0
Total Li (XRD/Reference)	18.0 / 17.2	18.7 / 18.5

Results of Rietveld refinement on Li_2CO_3 samples (3 σ in brackets).

Description and attachments

The design of the Thermo Scientific™ ARLTM X'TRA Companion is based on a vertical θ/θ Bragg Brentano geometry (160 mm radius) for convenient sample preparation and sample handling. It is the perfect companion for XRD qualitative and quantitative analysis of polycrystalline materials.

ARL X'TRA Companion operates at 600 Watts (copper or cobalt radiation) and an integrated water chiller is available. A precise control of the radial and axial collimation of the beam is ensured with mechanical slits, Soller slits and variable beam knife.



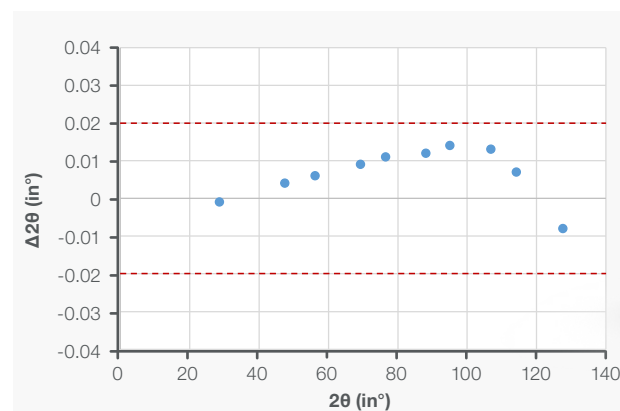
Schema of the geometry of the θ/θ goniometer.

The modular support design of the ARL X'TRA Companion allows users to exchange pre-aligned sample stages without requiring a lengthy realignment procedure.

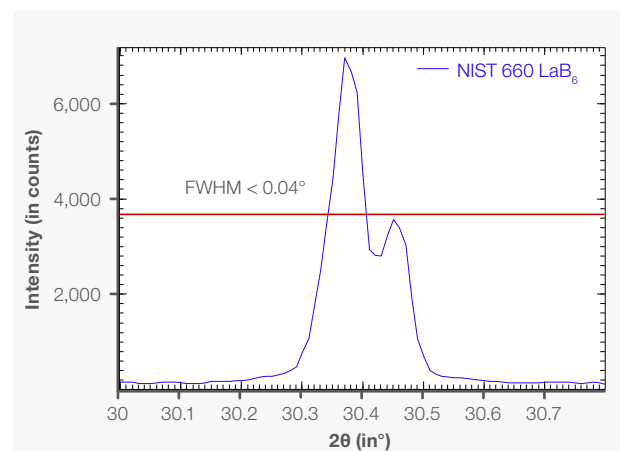
The standard sample stage incorporates one device that precisely orients both the translational and rotational orientation of the stage relative to the goniometer.

A reconfiguration of the diffractometer with a new sample batch is achievable in a few minutes.

The ARL X'TRA Companion provides very fast resolute data collection due to its state-of-the-art solid state pixel detector (55x55 μ m pitch) and it comes with one-click Rietveld quantification capabilities and automated result transmission to a LIMS.



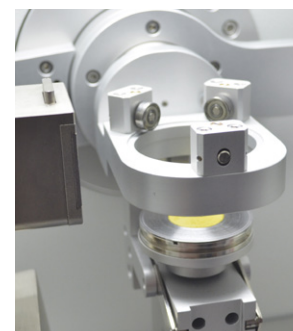
An angular accuracy better than $\pm 0.02^\circ$ over the whole 2θ range guarantees optimal instrument alignment to support accurate and reliable analysis. Test with a Si powder.



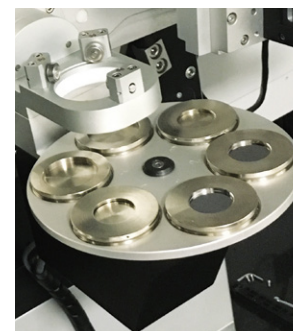
An angular resolution $< 0.04^\circ$ FWHM can be measured easily in standard configuration. Test with a LaB_6 powder.



ARL X'TRA Companion benchtop X-ray diffractometer.



Spinning sample stage.



6-position sample changer ϕ 51.5 mm (optional ϕ 40 mm version).

Complementary techniques Service

XRF and XRD

X-ray fluorescence (XRF) analysis determines the elemental composition of a sample but does not provide information about how the various elements are combined together. Such mineralogical information is only available through **X-ray diffraction** (XRD).

In a typical crystalline sample, XRF might measure, for example, the total Ca concentration or the total Fe concentration. XRD permits analysis of the phases or compounds in crystalline materials such as rocks, minerals, and oxide materials and products. In the same sample, XRD takes the analysis a stage further and gives information about CaO, CaCO₃, and Ca(OH)₂ content, and other Ca phases, or the levels of Fe phases, such as FeO, Fe₂O₃, Fe₃O₄, Fe₃C, and other Fe phases.

Therefore, combining the results of both XRF and XRD techniques allows for a better and more complete characterization of any given crystalline sample.



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ARL PERFORM'X
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ARL 9900
XRF/XRD

Customized solutions for peak performance

When you invest in Thermo Scientific measurement equipment, you not only benefit from product performance, you also enjoy peace of mind and maximum uptime with optimal service solutions provided. We offer a full suite of services and support designed to respond quickly and flexibly to diverse service needs and requests. Select only the service options you want or add them later for efficient, high-performance day-to-day use of your instrument.

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- Drive decisions and maximize instrument performance
- Reduce costs with increased production capability



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