



## Educating future professionals in XRD technique

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### Why teach XRD?

X-ray powder diffraction is a highly valuable characterization tool and a nondestructive technique for analyzing both organic and inorganic crystalline materials. Traditionally, this method has been employed for phase identification, quantitative analysis, and the determination of structural imperfections in samples from a variety of fields, including geology, polymer science, environmental studies, pharmaceuticals, and forensic science.

The challenge for educators lies in how to inspire, teach, and prepare the next generation of professional X-ray users and analysts for successful careers in this field.

### What are the principles of XRD?

X-Ray diffraction (XRD) is an effective and nondestructive method for identifying and quantifying the crystalline phase composition of both powdered and solid samples. This technique relies on the elastic scattering of photons by the atoms within a material. When these atoms are arranged in a periodic array, the scattered radiation experiences both destructive and constructive interference (diffraction) at particular angles. This phenomenon is explained by **Bragg's Law (Figure 1)**.

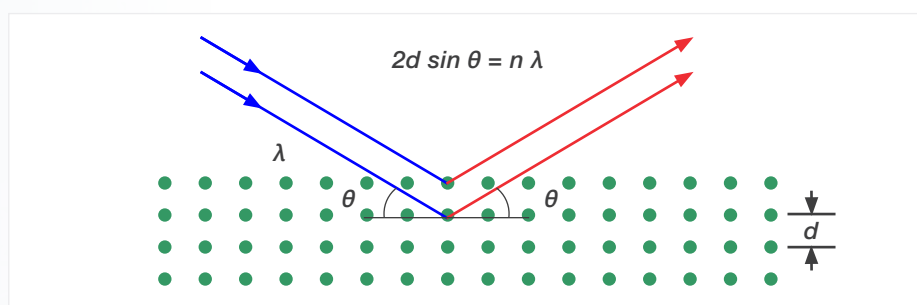


Figure 1. Bragg's law schema.

$\lambda$ : wavelength,  $d$ :  $d$  spacing,  $\theta$ : diffraction angle,  $n$ : diffraction order

The directions of the diffracted wave are influenced by the size and shape of the unit cell, while the intensities are determined by the atomic arrangement within the crystal. Consequently, a diffraction pattern can provide detailed information about the crystalline phases present (indicated by peak positions), the relative phase concentration (determined by the ratio of peak areas), the amorphous content (evident from background humps), and the crystallite size and strain (reflected in peak widths).

### What type of instrumentation is used?

The benchtop X-ray diffractometer, **Thermo Scientific™ ARL™ X'TRA Companion X-ray Diffractometer** (Figure 2), is the ideal companion for teaching X-ray diffraction (XRD). Robust, very safe, and easy-to-use, even for an inexperienced user, it enables the establishment of a simple and relevant experimental protocol for high-quality data acquisition in a short time. The results obtained are easily interpretable thanks to open-source software and free crystallographic databases.



Figure 2. ARL X'TRA Companion X-ray diffractometer system with  $\theta/\theta$  Bragg-Brentano geometry, perfect for all your educational and research needs

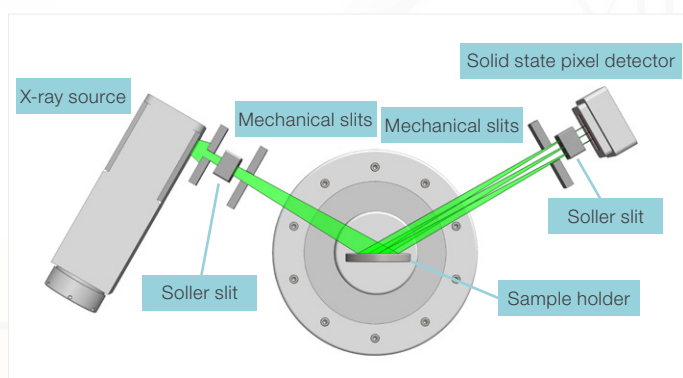


Figure 3.  $\theta/\theta$  geometry of the goniometer.

### What are these main characteristics?

The **ARL X'TRA Companion diffractometer** features a  $\theta/\theta$  goniometer (Figure 3) with a 160 mm radius in Bragg-Brentano geometry.

It is equipped with a 600 W X-ray source (available in either Cu or Co), and various sample supports tailored to the specific studied samples. The instrument could also include an integrated water cooler, making it fully autonomous.

Equipped with a state-of-the-art semiconductor pixel detector with a 55 x 55  $\mu\text{m}$  pitch, the **ARL X'TRA Companion diffractometer** enables very fast and high-resolution data collection, ensuring reliable data interpretation.

### What practical work would be possible?

#### Suggestion

Principles of X-ray diffraction and interpretation of data acquired on a given sample

#### Materials Needed

- ARL X'TRA Companion X-ray diffractometer (Figure 2)
- Sample holder with a crystal sample
- Computer with XRD analysis software

#### Methodology

1. **Introduce** the basic concepts of X-ray diffraction
2. **Explain** the setup and safety precautions
3. **Guide** students step-by-step

Start with sample preparation and show how to mount and align it on the sample holder.

Set up experiment parameters.

Start the experiment and monitor data collection.



Figure 4. Main software window.

1/ XRG menu, 2/ Motors status, 3/ Measurement status, 4/ Infos and errors, 5/ measurement setup.

#### 4. Data interpretation

Peak identification / Search match / Quantification (concept of the Rietveld method) / Crystal structure determination

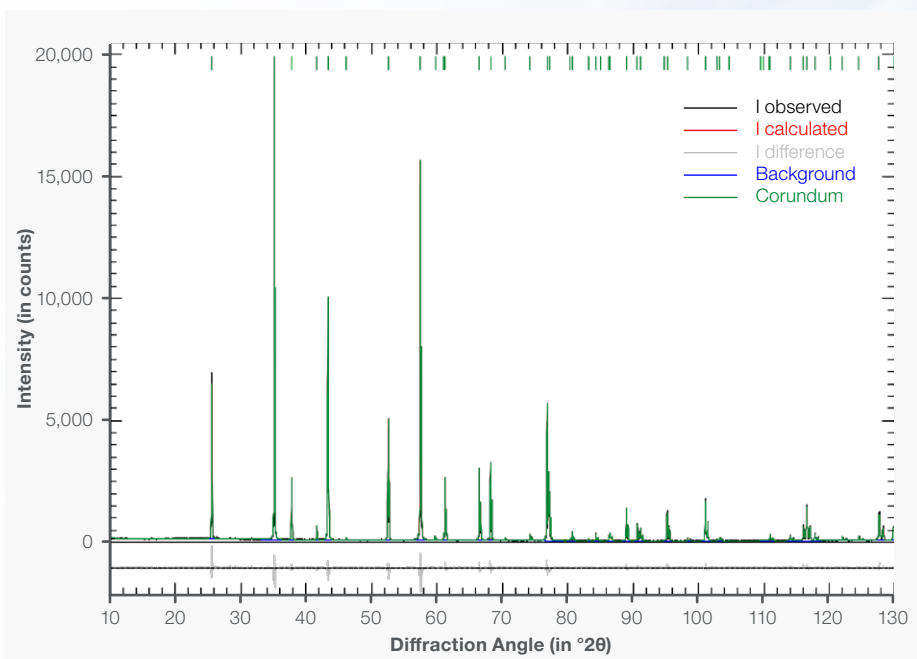


Figure 5. Alumina (NIST 1976) diffractogram.

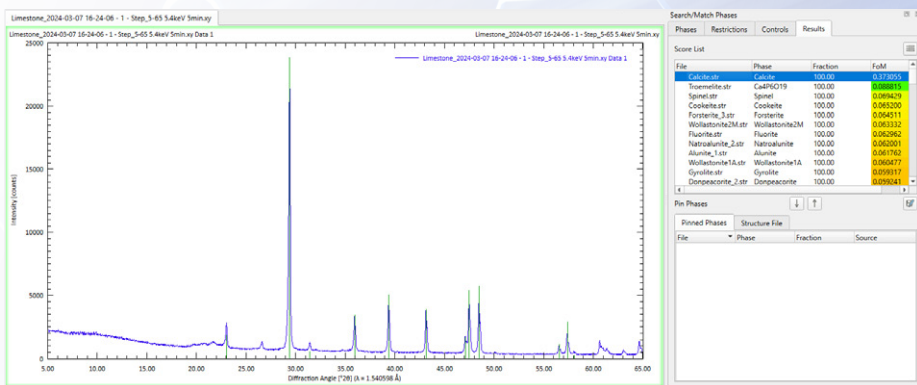


Figure 6. Result of a search-match analysis on a limestone sample with Profex software.

#### 5. Oral and written report

### What would be the minimal configuration of the ARL X'TRA Companion system for this work?

To ensure an optimal work with a minimal requirement, the configuration of the ARL X'TRA Companion system will be relatively simple:

- ✓ **ARL X'TRA Companion** benchtop XRD system
- ✓ Standard sample holder with a flat front-loading sample plate
- ✓ Computer
- ✓ Open-source Profex software for a free access to all students
- ✓ Free crystallographic databases access like COD (Crystallographic Open Database)

### What would be your conclusion about this XRD instrument?

The ARL XTRA Companion XRD benchtop system is specifically designed for use in student X-ray diffraction (XRD) laboratories. Its user-friendly interface makes it ideal for educational settings, offering hands-on experience with XRD techniques. This system enables students to conduct experiments focused on identifying and quantifying crystalline phases, analyzing diffraction patterns, and understanding the fundamental principles of X-ray diffraction.

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