X-Ray Powder Diffraction (XRD)

Principle:

X-ray diffraction analysis (XRD) is an analytical technique used for the identification of the crystallographic structure of a material and provide information on unit cell dimensions. It is based on constructive interference of monochromatic x-rays and crystalline sample.

XRD works by irradiating a material with incident x-rays and then measuring the intensities and scattering angles of the x-rays that leave the material. Crystals are regular arrays of atoms, whilst x-rays can be considered as waves of electromagnetic radiation. Crystal atoms scatter incident x-rays through interaction with the atoms' electrons. This phenomenon is called elastic scattering.

Current model:

Figure: Rigaku Miniflex 600 Benchtop XRD

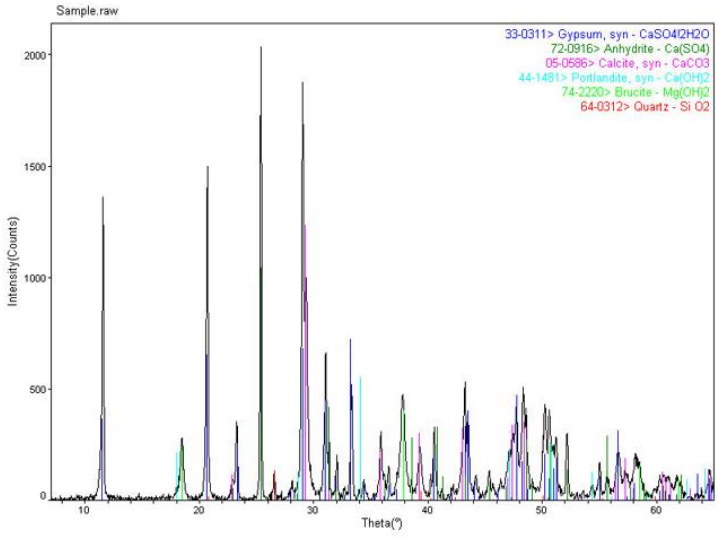
Video Link: https://www.rigaku.com/products/xrd/miniflex

X-ray diffractometers consist of three basic elements: X-ray tube, a sample holder, and an X-ray detector.

X-rays are generated in a cathode ray tube by heating a filament to produce electrons, accelerating the electrons toward a target by applying a voltage, and bombarding the target material with electrons. When electrons have sufficient energy to dislodge inner shell electrons of the target material, characteristic x-ray spectra are produced.

XRD can be used to determine structural properties such as lattice parameters, strain, grain size, epitaxy, phase composition and preferred orientation, measure thickness of thin films and multi-layers and determine atomic arrangement.

A summary table of analysis results and diffraction plot with reference pattern markers for visual comparison is shown below:



General X-ray diffraction phase identification and bulk elemental X-ray fluorescence are complimentary analyses, which provide elemental composition information and chemical phase and crystal structures actually present in a sample.

Typical samples:

Samples which are tested by XRD are crystalline materials such as minerals, clays, films, and inorganic compounds.

Standards:

Samples can be assessed in accordance with international standards such as: ATSM D3906 – 19 and ATSM D5357 – 19 or to customer requirements.

Contact: Dr Brendan Duffy, brendan.duffy@tudublin.ie, +353-1-220-6907