Author: Đoàn Hữu Nhân
National: Vietnam

POWDER X-RAY DIFFRACTION

1. WHAT IS X-RAY DIFFRACTION METHOD?

- X-ray diffraction analysis (XRD) is a technique used in materials science to determine the crystallographic structure of a material. 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.
- Bragg Law:
  - Diffraction will only occur if the way the x-rays and substance interact meets the conditions of Bragg's law:

$$n\lambda = 2d\sin\theta$$

where:

- λ is the wavelength of the x-ray,
- d is the spacing of the crystal layers (path difference),
- θ is the incident angle (the angle between incident ray and the scatter
- n is an integer

2. X-RAY DIFFRACTION INSTRUMENT?

- X-ray diffraction peaks are produced by constructive interference of a monochromatic beam of X-rays scattered at specific angles from each set of lattice planes in a sample when it is adapted to Bragg Law.
- The peak intensities are determined by the distribution of atoms within the lattice. Consequently, the X-ray diffraction pattern is the fingerprint of periodic atomic arrangements in each material
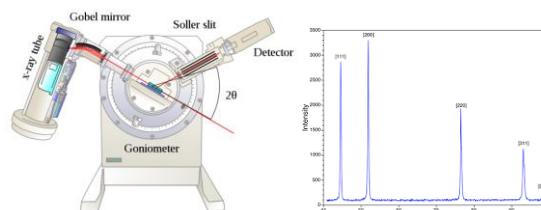
3. USING XRD FOR DETERMINE CRYSTALLINE STRUCTURE OF MATERIAL

3.1 CRYSTALLOGRAPHY OPEN DATABASE (COD):

- An open-access collection of crystal structures and platform for world-wide collaboration. The COD crystallographic database collects all crystal structures of 'small to medium sized unit cell' crystals—structures of organic, inorganic, metal-organic compounds, and minerals.
- COD data format form:

3.2 USING X'PERT HIGHSCORE SOFTWARE COMBINE WITH COD TO DETERMINE CRYSTALINE STRUCTURE:

HighScore (HC) is the ideal software for phase identification, semi-quantitative phase analysis, pattern treatment, profile fitting and more. HC helps is in getting fit the best powder diffraction (such as COD) pattern with our diffractometers patterns which scanned from XRD: