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A Review on X-Ray Diffraction

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ABSTRACT: X-Ray Diffraction (XRD) is a non-destructive technique that provides detailed information about the crystallographic structure, chemical composition, and physical properties of materials. 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. 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 a given material. This review summarizes the scientific trends associated with technique, instrumentation application of X-Ray Diffraction in the field of pharmaceutical industry, forensic science, glass industry, as well as in corrosion analysis.

KEYWORDS: Crystallographic structure,X-Ray Diffraction,Single beam

I. INTRODUCTION

[1]. X-Ray diffraction in crystals was discovered by Max von Laue in 1914. X- Ray Diffraction (XRD) is a non- destructive technique for analyzing the structure of materials primarily at the atomic or molecular level. It works best for materials that are crystalline or partially crystalline but it also used to study non-crystalline materials. X-Ray diffraction is quite different from X-ray radiography or Tomography. X-Ray diffraction produces a diffraction pattern, which does not superficially resemble the underlying structure and provides information about the internal structure on length scale from 0.1-100nm.[2]. It will analyze and identify unknown crystalline compounds by various method. The different parameters such as scan step size, collection time, range, X-Ray tube voltage and current should be fixed based on the specimen's requirement analysis. It is a rapid analyzing technique for phase identification of a crystalline material is finely ground, homogenized, and average bulk composition is determined. All diffraction method depends on generation of X-Rays in an X-Ray tube. The atomic planes of a crystal cause an incident beam of X-Ray to interfere with one another as they leave the crystal. The phenomenon is called as X-Ray diffraction. By this method one can identify crystal structure of various solid compounds. These methods are extremely important as compared with X-Ray absorption and X-Ray fluorescent method. X-Ray methods is mainly used in qualitative analysis, including structure elucidation of organic and inorganic compounds. Study of polymorphism in drugs is the pharmaceutical application by X-Ray diffraction technique. It can be applied as powder diffraction technique for the identification of fine - grained minerals.

II. ADVANTAGES

- It is a rapid band powerful technique for identifying unknown minerals and materials.
- [3] It only requires preparation of a minimal sample for analysis.
- Interpreting the resulting data is relatively straightforward.
- XRD measurements are widely available.

III. DISADVANTAGES

[4]. X-Rays do not interact very strongly with lighter elements.

IV. X-RAY DIFFRACTION METHODS

These are generally used for investigating the internal structure and crystal structure of various solid compounds. They are

1. Laue's photographic method
   - Transmission method
   - Black reflection method
2. Bragg's x-ray spectrometer method
3. Rotating crystal method
4. Powder method

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Transmission Laue Method

[5]. In this method the film is placed behind the crystal to record beams which are transmitted through the crystal. One side of the cone of Laue reflection is defined by the transmitted beam. The film intersect the cone with the diffraction spots generally lying on an ellipse. Can be used to orient crystal for solid experiments. Most suitable for the investigation of preferred orientation sheet particularly confined to lower diffraction angles. Also used in determination of symmetry of single crystal.

Black Reflection Method

[6]. In this method the film is placed between the x-ray source and the crystal. The beams which are diffracted in a backward direction are recorded. One side of the cone of Laue reflection is defined by the transmitted beam. The film intersects the cone, with the diffraction spot generally lying on a hyperbola. The method is similar to transmission method. Black reflection method is only for the study of large and thick specimens. Big crystal is required is considered as a disadvantage. Crystal orientation is determined from the position of the spot. Each spot can be indexed, using special charts. The Greninger chart is used for black reflection patterns. And the Leonhardt chart for transmission patter. The Laue technique can also be used to assess crystal perfection from the size and shape.

[7]. Laue beam of x-ray crystal emitted x-ray obtained on photographic plate using photograph bragg analyzed structure of crystal of NaCl, Kcl, and Zns-brag equation. Single plane generate several diffraction lines- sum tot of diffraction lined gives diffraction pattern from the pattern we can reduce different distance between plane angle between planes in each of three dimensions.

Powder crystal method

[8]. X-ray powder diffraction is a rapid analytical technique primarily used for phase identification of a crystalline material and can provide information on unit cell dimensions. The analyzed material is finely ground homogenized and average bulk composition is determined. Fine powder is struck on a hair with a gum, it is suspended vertically in the axis of a cylindrical camera.

V. APPLICATIONS OF X-RAY DIFFRACTION

- [9] Structure of crystal
- Polymer characterization
- State of anneal in metals
- Particle size determination
- Spot counting method
- Broadening of diffraction lines
- Low angle scattering
- Application in complexes
- Determination of cis and trans isomerism.
- Determination of linkage isomerism.
- Analysis of industrial dust.
- Study of corrosion product.
- Soil classification based observed crystallinity
- Linkage isomerism.
- [10] To identify crystalline phases and orientation.
- To determine structural properties:
- Lattice parameters (10-4Å), strain, grain size, epitaxy, phase composition, preferred orientation (Laue) order-disorder transformation, thermal expansion
- To determine atomic arrangement
- Detection limits: ~3% in a two-phase mixture; can be
- ~0.1% with synchrotron radiation Spatial resolution: normally none

VI. CONCLUSION

For materials including metals, minerals, plastics, pharmaceuticals and semiconductors X-Ray diffraction apparatus provide highly accurate tools for non- destructive analysis. The diffraction system are also supported by an extensive range of application software. To identify the crystalline phases present in a material and there by reveal chemical composition information. X-Ray diffraction is useful for evaluating polymers, corrosion products, and unknown materials. In the most cases the samples analyzed at element are analyzed by powder diffraction using samples prepared as finely ground powders. X-Ray diffraction is extremely efficient for the characteristics of the sample due to data acquisition is straight forward and short set up time is required. Spectra obtained are simple and easy to interpret. X-Rays are not much absorbed by air, so the specimen need not to be in an evacuated chamber.X-Ray diifraction has provided a wealth of important information for science and industry. The arrangement and spacing of atoms in crystalline material has been determined directly from diffraction studies. The distance between atom in crystals have been found to be roughly equal to 10 cm. So optical and electron microscope cannot be used this field. Synctron X-Ray

diffraction was developed which is similar in design to conventional X-Ray diffraction. So the X-Ray diffraction is limited to crystalline materials.Study of polymorphism is the pharmaceutical application of X-Ray diffraction.X-Ray Diffraction patterns are available in the database and can be compared for easy interpretation.Measurements of thickness of thin films and multi layers can be done by X-Ray diffraction technique.X-Ray diffraction pattern can be interpret by forensic science , so X-Ray diffraction technique has a major role in the forensic science.

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