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Applications of X-Ray Diffraction in Civil Engineering

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Abstract: *X-ray diffraction (XRD) is a robust non-destructive technique for characterizing crystalline materials. It provides data on structures, phases, most well-liked crystal orientations (texture), and various structural parameters, like average grain size, crystallinity, strain, and crystal defects. XRD peaks are made by constructive interference of a monochromatic beam of X-rays scattered at specific angles from every set of lattice planes in the sample. The intensities of peak intensities are determined by the distribution of atoms inside the lattice. Consequently, the diffraction pattern is the fingerprint of periodic atomic arrangements in a very given material. This review summarizes the scientific trends related to the fast development of the technique of diffraction over the past 5 years touching on the fields of prescribed drugs, rhetorical science, geologic applications, micro-electronics, and glass producing, also in corrosion analysis.*

Key Word*: Structures, lattice, X-ray diffraction.*

I. INTRODUCTION

Max von Laue and Co., in 1912, discovered that crystalline substances act as three-dimensional optical phenomenon gratings for X-ray wavelengths almost like the spacing of planes in a Bravais lattice. X-ray diffraction is currently a commonly used technique for the study of crystal structures and atomic spacing. X-ray diffraction is predicated on constructive interference of monochromatic X-rays and a crystalline sample. These X-rays are generated by a tube of cathode ray, filtered to yield monochromatic radiation, collimated to concentrate, and focused toward the sample. The interaction of the incident rays with the sample produces constructive interference once conditions satisfy Bragg's law: $n\lambda=2d\sin\Theta$ where n is an integer, λ is the wavelength of the X-rays, d is the inter-planar spacing generating the optical phenomenon of diffraction, and u is the diffraction angle. This law relates the wavelength of electromagnetic wave to the diffraction angle and therefore the lattice spacing in a very crystalline sample. These diffracted X-rays are then spotted, processed, and counted. By scanning the sample through a spread of 2u angles, all achievable diffraction directions of the lattice ought to be realized due to the arbitrary orientation of the powdery material. Conversion of the diffraction peaks to d-spacings permits identification of the compound as a result of every compound features a set of distinctive d-spacings. Typically, this can be achieved by comparison of d-spacings with standard reference patterns. X-ray diffractometers carries with it 3 basic elements: An X-ray tube, a sample holder, and X-ray detector. X-rays are generated in a tube of cathode ray by heating a filament to produce electrons, accelerating the electrons towards a target by applying a voltage and bombarding the target material with electrons.

X-ray diffraction is a robust laboratory technique often used in conjunction with microscopy and chemical analysis during materials characterization and failure investigations of construction materials.

- Determination of bulk mineralogical composition of a concrete or mortar, including its aggregate and binder mineralogy's; e.g.,
    - Quartz in sand, or
    - Calcite in sand or carbonated lime binder, or
    - Portlandite in binder;
- Individual mineralogy and alteration products of aggregates at varied size fractions, and binder phases;
- Detection of dolomitic lime binder from brucite within the mortar;
- Detection of gypsum, lime (Portlandite), or cement binders;
- Detection of any possibly deleterious constituents, e.g., deleterious salts, or efflorescence deposits;
- Detection of a mineral oxide-based pigmenting constituent; and,
- Detection of components, which are difficult to detect by microscopically ways.

Fig. 1.: X-Ray Diffractometer

Fig 2 (a).: *Test Sample*

Fig 2 (b).: *Working on XRD Machine*

Fig 2(c).: *Slits*

Fig 2 (d): *Chiller*

Fig 2 (e) *Toolkit*

II. STRENGTHS AND LIMITATIONS

Strengths:

1. Powerful and rapid (less than 20 min) for identification of an unknown mineral.
2. Provides unequivocal mineral determination in maximum cases.
3. Requires minimal sample preparation.
4. Wide availability of XRD units.
5. Relatively straightforward data interpretation.

Limitations:

1. Homogeneous and single-phase material is best for identification of an unidentified.
2. Access to a standard reference file of inorganic compounds is prerequisite.
3. Material, in one-tenth of a gram quantity, must be crushed into a powder
4. For mixed materials, detection limit is 2% of sample.
5. For unit cell determinations, indexing of patterns for non- isometric crystal systems is intricate.
6. Peak overlay may arise and deteriorates for high angle "reflections".

X-ray diffraction is a high-tech, non-destructive technique for analyzing a wide range of materials including fluids, metals, minerals, polymers, catalysts, plastics, pharmaceuticals, thin-film coatings, ceramics, solar cells, and semiconductors. The technique identifies countless practical applications in various industries, including microelectronics, power generation, aerospace and many others. XRD analysis can easily detect the presence of defects in a particular crystal, its resistance level to stress, its texture, its size and degree of crystallinity, and virtually any other variable component relating to the sample's basic structure.

The objective of this review is to present the new advances in applications of XRD in diverse analysis, covering the duration between 2009 and 2014. It is useful to give a short introduction to the concept of the XRD, some features of the instruments used, and sample preparation. Quantitative and qualitative determination in various fields of analysis using this method will be presented.

III. XRD THEORETICAL ASPECTS

Instrumentation

The instrument arrangement that is used for measurements of powder diffraction has not altered much from that advanced in the late 1940s. The key change found in modern-day instrumentation is the use of the minicomputer for control, data acquisition, and data processing. Fig-2 illustrates the geometry of the system, showing the layout of a typical diffractometer with system source Soler-slits P and RP, sample S divergence slit D and receiving slit R

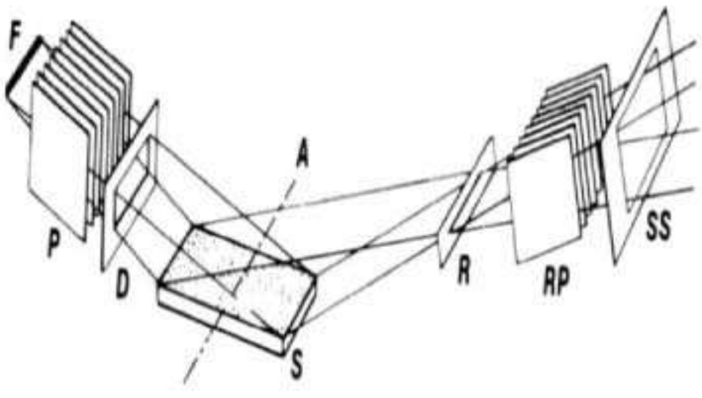

Fig. 3.: *Geometry of the Bragg-Brentano diffractometer*

Application of XRD in Cement (Mineralogical diversity in natural cement)

Contrary to Portland cement that comprises four common phases, alite, belite, aluminate, ferrite, and, the set-controlling phase, gypsum, natural cements (due to comparatively low-temperature calcination) hold a large number of phases from several degrees of calcinations all of which can be recognized by XRD:

a) Calcined, air-slaked, and un-calcined produces of calcite in limestone i.e., free lime, portlandite, and calcite, respectively;
b) New minerals made from calcination and lime-silica reactions viz. periclase and larnite, respectively;
c) Original phases from raw feed that has not been calcined or reacted, e.g., dolomite, calcite, and quartz;
d) Added set-controlling phases, e.g., anhydrite, gypsum, bassanite.

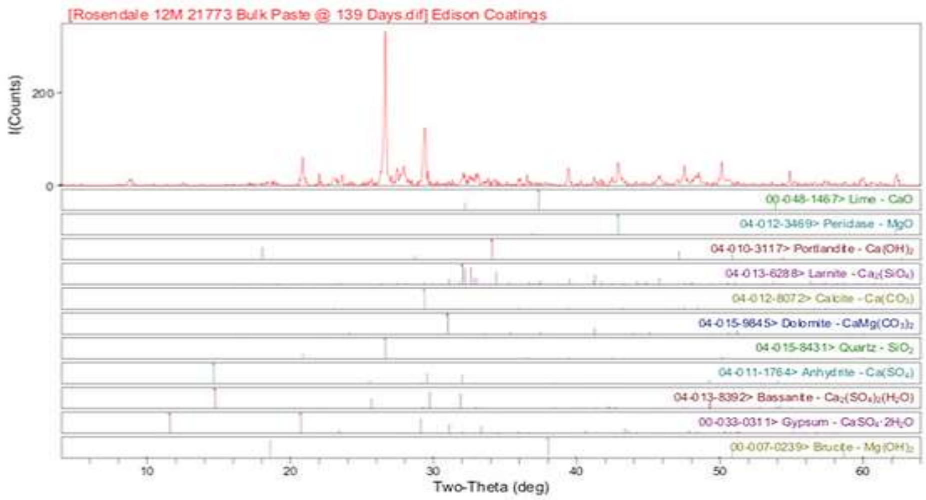

Fig. 4.: *Graph Analysis*

Application of XRD in Cement Manufacturing
(Mineralogical variations during consecutive heating of a dolomitic limestone raw feed to yield natural cement)

Quantitative determination of several minerals from XRD – lessening calcite, dolomite, and quartz matters in the calcined raw feed at the cost of free lime, periclase, and larnite formation in natural cement:

(a) Dolomitic limestone is raw feed at room temperature:
Free Lime – 0.0%, Periclase – 0.0%, Portlandite – 1.0%, Larnite – 2.8%, Calcite – 39.3%, Dolomite – 32.9%, Quartz – 17.4%

(b) Calcined dolomitic limestone at 600 degrees Celsius:
Free Lime – 0.0%, Periclase – 1.1%, Portlandite – 0.8%, Larnite – 3.4%, Calcite – 54.1%, Dolomite – 17.3%, Quartz – 15.7%

(c) Calcined dolomitic limestone at 900 degrees Celsius:
Free Lime – 23.8%, Periclase – 17.8%, Portlandite – 2.3%, Larnite – 46.7%, Calcite – 0.0%, Dolomite – 3.0%, Quartz – 2.8%

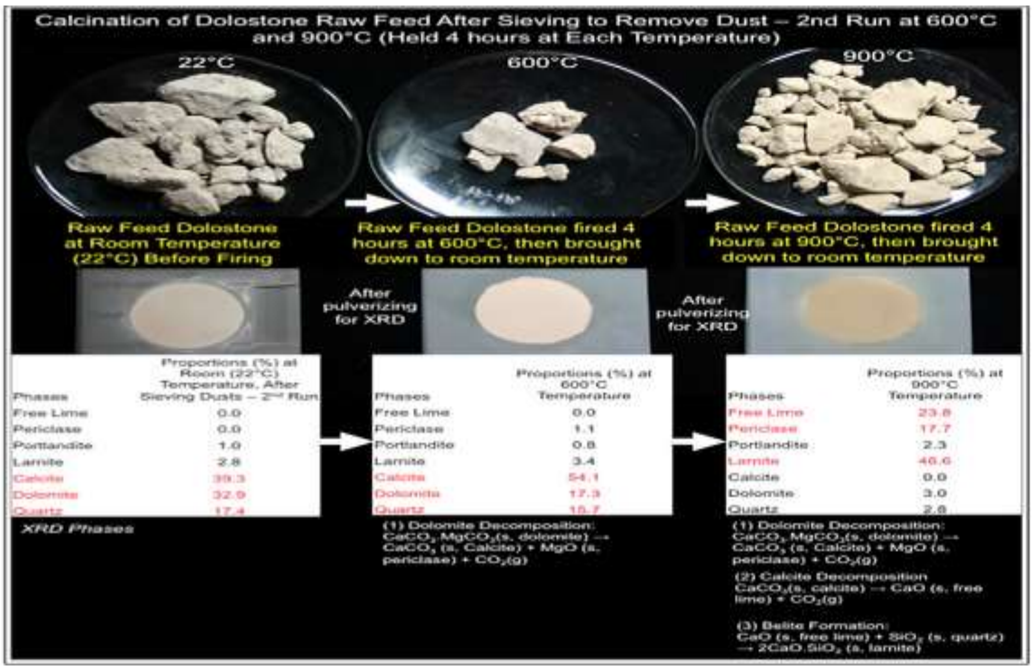

Fig. 5.: *Calcination of Dolostone*

Application of XRD in Concrete

1. Aggregate mineralogy
2. Unsound constituents in aggregates
3. Efflorescence salts
4. Cement hydration products
5. Cement minerals
6. Contaminants
7. Bulk mineralogy of concrete

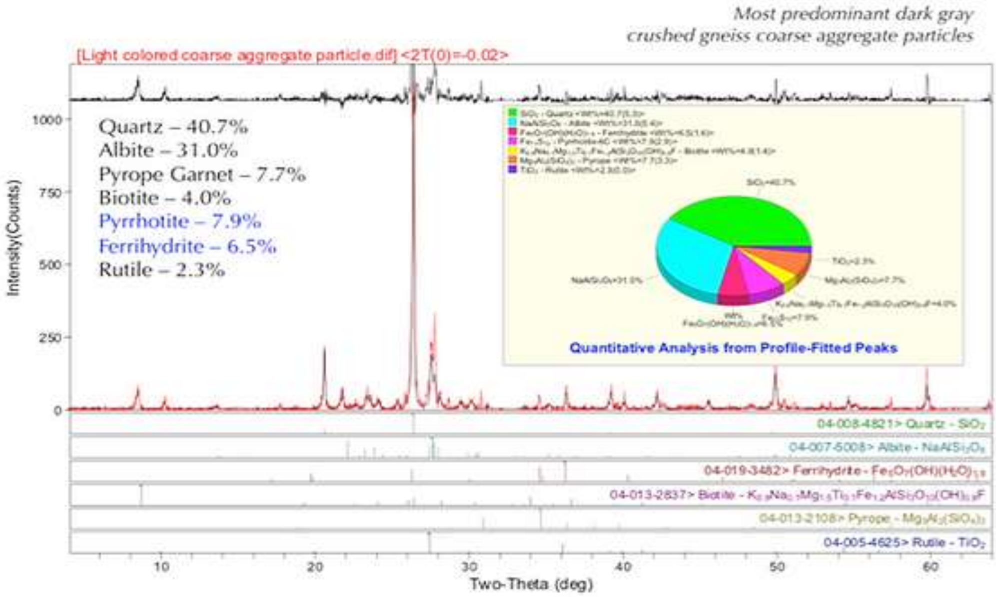

Fig. 6.: *Qualitative Analysis*

Application of XRD in Historic Masonry

1. Mortar from Fort Zachary Taylor, FL
2. Extensive Salt Contamination
3. Marine Shell as Sand
4. Sodium Chloride or NaCl (41.6%) from Mixing Mortar with Sea Water
5. Equal Calcite and Aragonite (each 25-30%) from Carbonated Lime Matrix, and Sea Shells, respectively
6. Minor Quartz from Contaminant

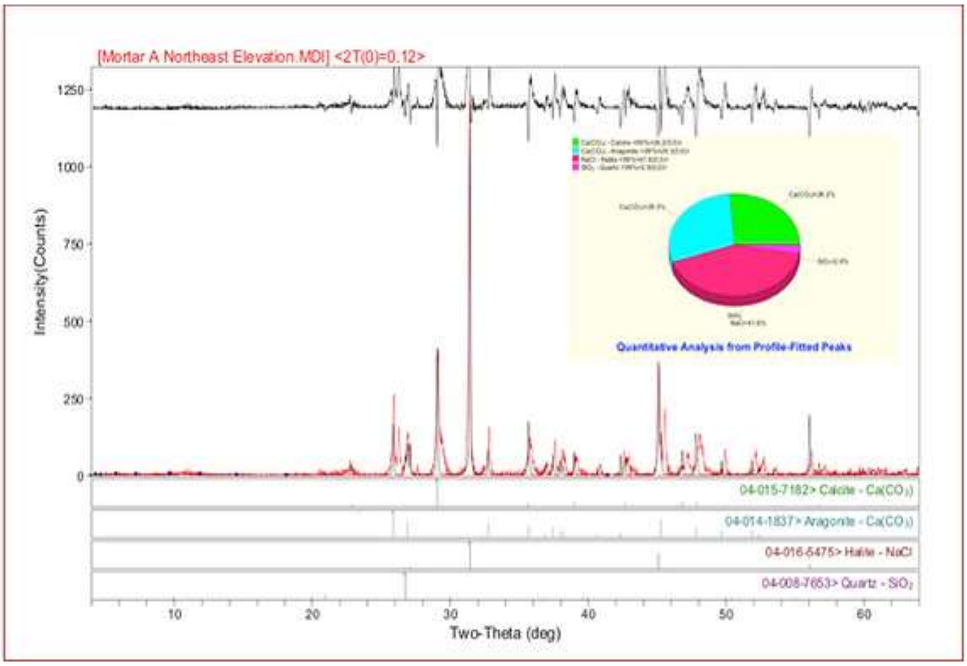

Fig. 7.: *Graph Analysis*

IV.CONCLUSION

X-ray diffraction (XRD)is an analytical technique used to characterize crystalline phases of a wide variety of materials, typically for mineralogical analysis and identification of unknown materials. Powder diffraction data are basically derived by the atomic and molecular arrangements described by the physics of crystallography. There are several advantages of XRD techniques in science laboratories: Nondestructive, fast, and easy sample preparation High-accuracy for d-spacing calculations Can be done in situ permits characterizing single crystal, poly, and unstructured materials Standards are obtainable for thousands of material systems. In the early years, powder XRD systems have become more and more effective for the pharmaceuticals sector due to innovations and improvements in detection and source emission technology. X-ray diffraction methods are especially substantial for the analysis of solid materials in forensic science. They are often the only procedures that allow a further differentiation of materials under laboratory conditions. Minerals are characterized as building blocks of the solid Earth. Some minerals are readily recognized by their unique colors or crystal forms, but in most cases, powder X-ray diffraction is the primary and most definitive method used to identify minerals. The high flux and density of X-rays produced at synchrotrons offer the micro-electronics industry with a potent probe of the structure and behavior of a wide range of solid materials that are being advanced for use in devices of the future. X-ray diffraction studies are also used to acquire data on the short and intermediate range structure of glasses.

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