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Research Article

Python Based Property Evaluation of Co-Zn Ferrite: Using results of XRD and FTIR

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Abstract

The study focuses on making a new material by mixing different combinations of cobalt, zinc, and iron with sodium hydroxide. These formed materials are known as ferrite. The main goal of this study is to investigate how the properties of synthesized ferrite change as we change the composition. These types of ferrites have practical uses in industries like electronics, magnets, nuclear energy sector, and healthcare. By understanding how various variations in material's composition affect the properties of material researchers can design materials which have higher efficiency and greater longevity. Based on the result of the above study this research presents a further investigation into the analysis of Co-Zn substituted ferrite nanoparticles by applying advanced data analytics using Python. Python allows for statistical evaluation, processing and modeling, as well as visualization of XRD for structural analysis of material and FTIR data for functional group analysis of material. Different aspects of XRD analysis

cover the intensity vs. 2Theta spectrum visualization which gives various information about composition of material, identification of peaks, Scherrer methodbased crystallite size estimation, and determination of lattice parameters. FTIR techniques involve spectral peaks identification, functional groups assignment, and an estimation of the material's band gap. The integration of these technologies provides an improved understanding of spinel phase formation, nanoparticle size distribution, and other structural changes in material. By integrating FTIR analysis, peak detection, functional group identification, and FWHM-based crystallite size estimation, we can obtain better interpretation of experimental data, which leads to enhanced insights into material properties. This procedure contributes significantly to advancing research in nanoscience and the thorough characterization of synthesized materials.

Keywords: Ferrite, Co-Zn, X-ray diffraction [XRD], Fourier transform infrared [FTIR], Nanoscience, Python.

1. Introduction

The materials which are formed by combining oxygen with two or more elements and after formation they have their own chemical composition in which the element that has higher number of bonds with oxygen belongs to the special category of polymetallic oxides is ferrimagnetic oxide. This material is known as ferrite. There are different types of ferrites such as Nickel-Zinc (Ni-Zn) Ferrite, Manganese-Zinc (Mn-Zn) Ferrites, Magnesium-Zinc (Mg-Zn) Ferrites, Cobalt - Zinc (Co-Zn) Ferrite etc. For our study we have used Cobalt-Zinc (Co-Zn) Ferrite.

Co-Zn ferrites belong to spinal ferrites which are a class of chemically and thermally stable materials suitable for a wide variety of applications. Ferrites have numerous advantages as compared to other type of magnetic materials, they have high electrical resistivity, high permeability and due to its time/temperature stability use of ferrites is increased in quality filter circuits, wide-band transformer and various high frequency electronic circuitry. Also, they can be used in magnetic devices, humidity sensors and gas sensors. Co-Zn ferrite has the ability to fight bacteria, particularly Escherichia coli (E. coli), which is a common waterborne pathogen. It can be used to disinfect water by killing harmful bacteria and it is a unique approach to improve water treatment methods. This Co-Zn ferrite was further tested using two X-Ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR).

X-Ray diffraction (XRD) is a fast analytical technique based on Bragg's law ($n\lambda = 2d\sin\theta$) which is mainly used for phase determination of crystalline material and it can also provide details about unit cell dimensions of crystal. This technique is very useful in identifying unknown crystalline materials and it is a non-destructive technique. A monochromatic beam of X-rays is incident on a material, and reflected X-rays are detected by a detector. Some of the incident beams of X-rays are partly absorbed, partly scattered, and the rest is transmitted unchanged through the material. The scattering occurs due to interaction between the incident

X-ray beam with the electrons in the material, and the diffracted X-rays interact with each other to cause diffraction patterns that depend on the angle of the incident beam in relation to the material. The diffraction pattern which is obtained from XRD Technique can be used as "Fingerprints" to determine the crystalline phase.

Fourier transform infrared (FTIR) spectroscopy is method in which absorption and transmission of infrared radiation takes place by material. Based on this data the spectrum is created which is basically molecular fingerprint of material. This fingerprint presents the absorption peaks generated by different components of the material which gives information about composition of material. In FTIR the IR radiations are passed through material. Some of the radiations are absorbed some passed through it (transmitted). The spectrum describes the presence of various chemical bonds and functional group present in the material. The FTIR is a non- destructive chemical imaging technology. The spectrum obtained from FTIR describes the distribution of molecules or functional groups. For characterization of material down to few microns area the FTIR is a rapid and accurate method. FTIR spectroscopy is carried out for identifying the composition and purity of materials also to study the chemical structure of materials. This spectroscopy provides in-depth information about the molecular composition and chemical bonding, which is useful for analyzing the structure and properties of a particular material.

Further we are leveraging the data analysis capacities of Python because of its advanced capabilities in statistical analysis, data processing and visualization. With advance libraries like Numpy, Scipy, Matplotlib lib etc. that efficiently handles large and complex data sets enabling statistical and computational analysis. In XRD (X-ray Diffraction) structural analysis python helps visualizing intensity VS 2Theta spectra which will in turn allow an in-depth research to the researchers to study the material composition. It facilitates the peak identification, Scherrer method based crystalline size estimation and lattice parameter determinations all which are essential to comprehend the concept of material science. Similarly, for FTIR (Fourier Transform Infrared Spectroscopy) it provides peak detection, functional group assignment and band gap estimation making it easier to comprehend the chemical properties of material.

Python libraries that we are using are Matplot lib for graphical representation of the result, Pandas for processing the .csv and .dpt file that converts raw data into structured data frame, NumPy to handle the numerical computations throughout our analysis. It is responsible for converting data columns to numerical values and performing key mathematical operations including the Scherrer equations that estimates crystalline size and SciPy for advance signal processing specifically the find_peaks() And peak() widths() functions. The find_peaks() plays an Important role in identifying peaks in both XRD and FTIR spectra, which is essential for crystalline size estimation and functional group analysis. Meanwhile, peak_widhs() calculates the full width at half maximum a key parameter in determining crystalline size.

Section 2 contains Literature review, Section 3 contains Methodology, Section 4 contains Result analysis, Section 5 contains Conclusion and Section 6 contains Glossary for the research paper.

Advantages of using python :-

- Time efficient.
- Rapid data processing for large datasets.
- Precision in numerical computation.
- Consistency in result for various datasets.
- Reduction in manual efforts and errors.

2. Literature review

D. D.Kulkarni, D. H. Kelkar, and K. P. Bodas (2023) discussed the vast applications of ferrites in electronics, high-frequency devices, biotechnology, and power systems (Kulkarni et al., 2023). Because of ferrites' certain characteristics, such as its electrical resistivity and the chemical stability, they excel in several fields. These characteristics has played a crucial role in the development of electronic circuits and biomedical applications as well . The XRD analysis shows the maximum reflection occurs from the (35) plane, which indicates the spinel phase. A broad XRD line indicates particles within the nano-size range. The peaks of absorption at 600 cm^{-1} and 400 cm^{-1} also ensure the existence of tetrahedral and octahedral groups (Kulkarni et al., 2023).

IIT Kharagpur and other institutions' research (ScienceDirect, 2021; Central Research Facility, IIT Kharagpur, 2021) identifies the use of X-ray Diffraction (XRD) for phase identification and structural characterization. Bragg's Law and Scherrer's Equation are essential applications in finding crystal size.

Pacific Bio-Lab, Specac, and other authors (Pacific Bio-Lab, 2022; Specac, 2022) highlighted the importance of Fourier Transform Infrared (FTIR) Spectroscopy as a crucial method for characterization of ferrite nanoparticles, which are commonly used for identification of molecular structure and functional groups.

Department of Chemistry and Biochemistry, University of California & University of Wisconsin–Madison (Wisconsin-Madison, 2015) indicated that absorption peaks between 400–600 cm^{-1} validate the existence of tetrahedral and octahedral sites in ferrite structure.

B. Patil (2022) investigated the correlation between synthesis conditions and functional properties and asserted that reaction temperature, pH, and synthesis parameters directly affect magnetic and electrical properties of ferrite materials.

According to studies ferrites can be grouped into various kinds such as Nickel-Zinc (Ni-Zn), Manganese-Zinc (Mn-Zn), Magnesium-Zinc (Mg-Zn), and Cobalt-Zinc (Co-Zn) ferrites.

Co-Zn ferrites has drawn a significant interest for their antibacterial property and prospects in water treatment (Zhukov, 2012; Mandal, 2016).

GeeksforGeeks (2021) emphasized the use of Python libraries such as NumPy, SciPy, and Matplotlib in spectral analysis that enhances the peak detection and minimizes human errors.

3. Methodology

XRD Characterization obtained from CFC Department, Shivaji University.

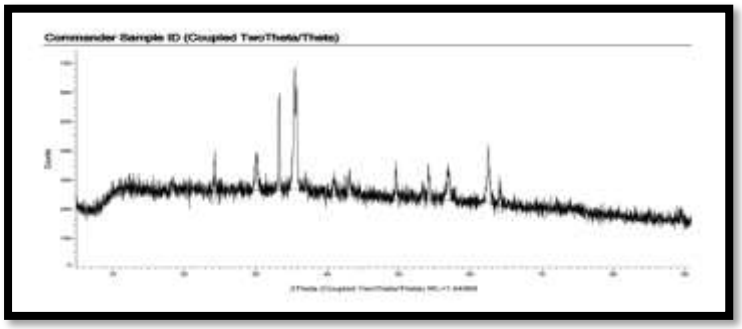


Figure 1 X-Ray Diffraction of Co0.1Zn0.9Fe2O4

FTIR Characterization obtained from CFC Department, Shivaji University.

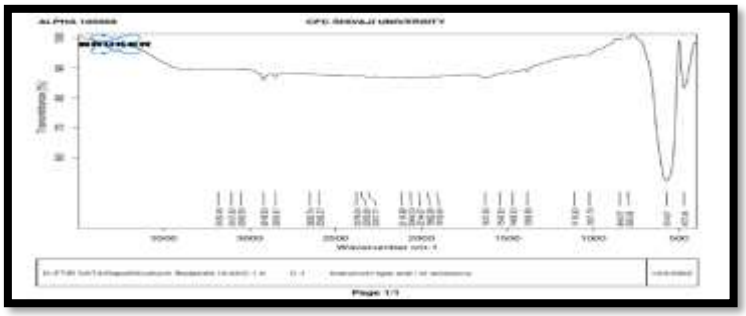


Figure 2 FTIR of Co0.1Zn0.9Fe2O4

XRD Characterization and Calculation using Python.

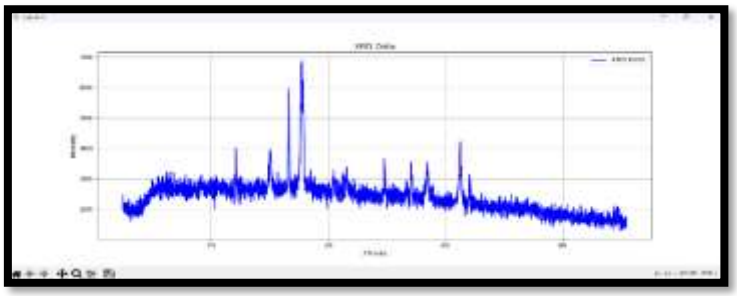


Figure 3 X-Ray Diffraction of Co0.1Zn0.9Fe2O4 using python.

The X-ray diffraction (XRD) pattern for C-1 exhibits sharp diffraction peaks, indicating its

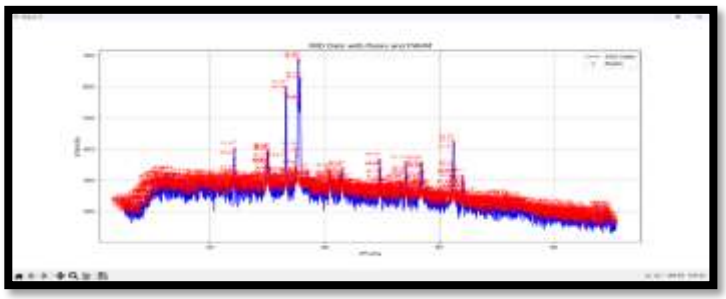
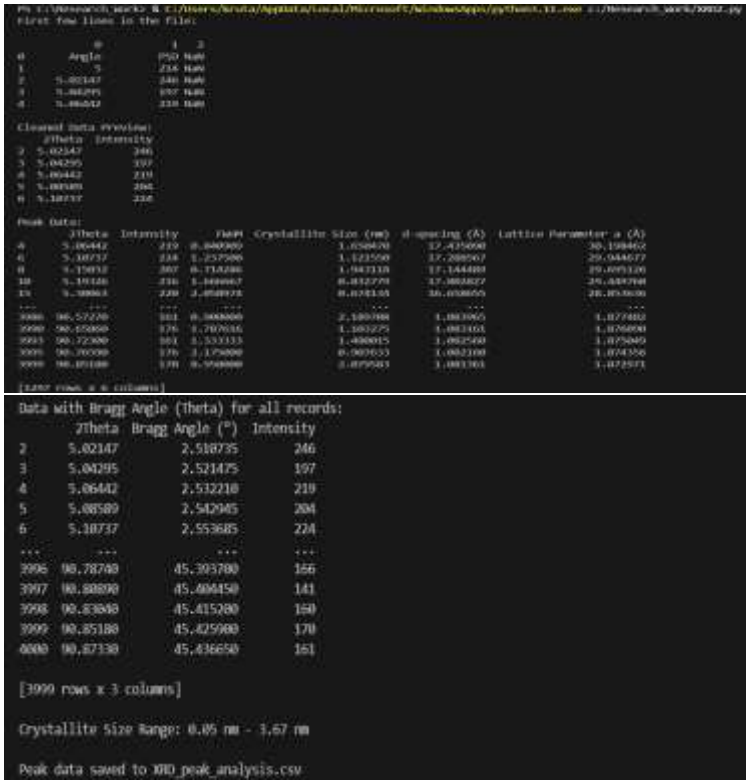


Figure 4 X-Ray Diffraction with Peak Detection and identification of FWHM of Co0.1Zn0.9Fe2O4 using python.

polycrystalline nature. The prominent peaks observed at 35.49°, 33.24°, and 62.55° correspond to the Co-Zn spinel ferrite phase, confirming the material's structural identity. The calculated crystalline size determined using the Scherrer equation, ranges between 0.07 nm to 3.55 nm. These results confirm the successful synthesis of a nanocrystalline material with a well-ordered crystalline structure.



Data with Bragg Angle (Theta) for all records:

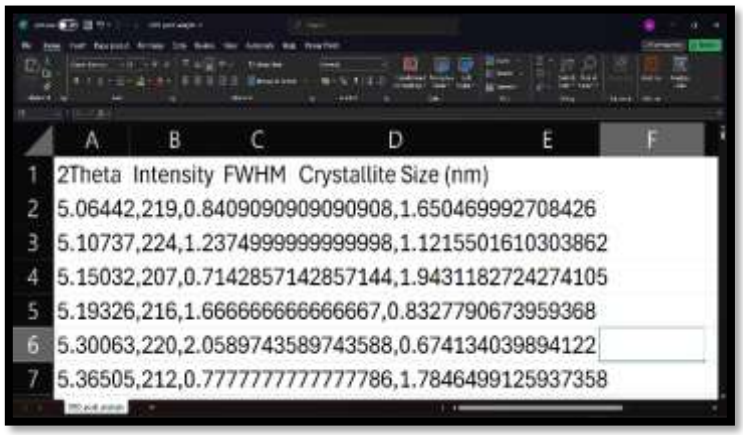
	2Theta	Bragg Angle (°)	Intensity
2	5.02147	2.510735	246
3	5.04295	2.521475	197
4	5.06442	2.532210	219
5	5.08589	2.542945	204
6	5.10737	2.553685	224
...	...	...	...
3996	90.78700	45.393700	166
3997	90.80890	45.404450	141
3998	90.83040	45.415200	160
3999	90.85180	45.425900	170
4000	90.87330	45.436650	161

[3999 rows x 3 columns]

Crystallite Size Range: 0.05 nm - 1.67 nm

Peak data saved to XRD_peak_analysis.csv

Figure 5 Output of Calculated properties of Co0.1Zn0.9Fe2O4 in python terminal.



	A	B	C	D	E	F
1	2Theta	Intensity	FWHM	Crystallite Size (nm)		
2	5.06442	219	0.8409090909090908	1.650469992708426		
3	5.10737	224	1.2374999999999998	1.1215501610303862		
4	5.15032	207	0.7142857142857144	1.9431182724274105		
5	5.19326	216	1.666666666666667	0.8327790673959368		
6	5.30063	220	2.0589743589743588	0.674134039894122		
7	5.36505	212	0.7777777777777786	1.7846499125937358		

Figure 6 Excel sheet of calculated properties of XRD.

FTIR Spectrum and Calculation using Python.

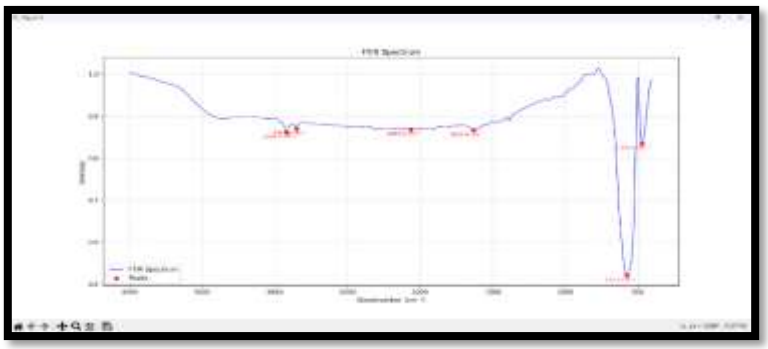


Figure 7 FTIR of Co0.1Zn0.9Fe2O4 using python

Figure 8 Output of Calculated properties of Co0.1Zn0.9Fe2O4 in python terminal.

The FTIR analysis of Co0.1Zn0.9Fe2O4 states the presence of alkanes, aromatics and possible carboxylic acids in sample based on the characteristic's absorption peaks. The peaks 2920.5 cm^{-1} and 2851.2 cm^{-1} demonstrates C-H stretching (alkanes) while the 1631.6 cm^{-1} suggests that C=C stretching (aromatics) or N-H bending (amides). Peaks at Peaks at 2920.58 cm^{-1} and 2851.16 cm^{-1} aligns with the O-H stretching in the carboxylic acids which indicated their presence. The FTIR spectrum visually reinforces these findings, highlights absorption in the 2800-3000 cm^{-1} and 1631.6 cm^{-1} regions. These results provide a valuable insight into the sample's chemical composition and structural characteristics. Based on the calculation the estimated band is 2447.35cm^{-1}. For identified peaks width of particular peak is calculated and shown in the python terminal.

4. Result Analysis

3.1 X-Ray Diffraction (XRD) result analysis

XRD or X-ray Diffraction is an essential procedure used for analyzing the crystallographic structure of materials. The code that we have for our analysis processes the XRD data in the .txt files where the 2Theta values and corresponding intensity measurements are recorded. The data is first cleaned by

$$D = K \lambda / \beta \cos(\theta)$$

removing the metadata rows and non-numeric entries ensuring an accurate representation of the diffraction patterns. The function find_peak () is used to detect the significant diffraction peaks in XRD spectrum. These peaks correspond to Bragg reflection that are crucial for determining crystalline size and lattice parameter. The code follows the Scherrer equation to estimate crystalline size (D) which is defined as :-

Equation 1

Where K is the Scherrer constant (typically 0.9), λ is the X-ray wavelength (Cu-Kα, 1.5406 Å), β is the full width at half maximum (FWHM) of the peak in radians and θ is the Bragg angle (half of the 2Theta value at the peak position). The peak_width () function calculates FWHM values to facilitate this estimation. Moreover, the interplanar spacing (d- spacing) is calculated using Bragg's law given by :-

$$d = \lambda / 2 \sin(\theta)$$ *Equation 2*

for materials with a cubic crystal structure, the lattice parameter (a) is determined by :-

$$a = d * \sqrt{h^2 + k^2 + l^2}$$ *Equation 3*

where h, k, l are miller indices of the diffraction planes. Then these calculations are performed in the code and tabulated for further analysis. The processed XRD data is then visualized using the matplotlib library where the 2Theta is plotted on the X-axis and intensity is plotted on the Y-axis. The detected peaks are marked with their respective 2Theta values and saved in the CSV file for documentation. This automated way enhances the efficiency and accuracy of the phase identification, crystalline size estimation and the lattice parameter determination making it valuable for the characterization of materials such as Co-Zn substituted ferrite nanoparticles.

3.2 Fourier transform infrared (FTIR) spectroscopy result analysis

Our python code has a data set stored in a .dpt file that contains wavenumber (cm^{-1}) and intensity (absorbance or transmittance) values. The function read_dpt_file () in our code extracts and organizes the spectral data (Data representing the intensity of light) ensuring that only valid numerical entries are considered for the analysis. Furthermore, to interpret the spectrum we have used the peak detection and functional group identification. The identity_peak() function applies to the find_peak algorithm from the SciPy library to detect absorption bands based on prominence, that in turn helps in the identification of characteristic vibrational modes. These detected peaks are then cross-referenced with the known absorption ranges using the function functional_group_identification that associates the absorbed wavenumbers with specific chemical functionals groups such as O-H (Hydroxyl group i.e.

Alcohols, Phenols , Carboxylic Acids) , C=H (i.e. Alkanes , Alkenes, Aromatics), N-H (Amines, Amides) and C=C (Alkenes, Aromatic Compounds).

Moreover, the quantitative analysis is performed using full width at half maximum (i.e. FWHM) measurements through the measure_peak_widths() function. The FWHM values provide better insights into the sharpness and broadening of spectral peaks, which is influenced by factors such as crystallinity molecular interaction and instrumental resolution. Additionally the code estimates the band gap energy from spectral data using the calculate-band_gap( ) that is relevant for the materials exhibiting the semiconductor behavior.

For the material classification identify_substance( ) function compares the detected FTIR peaks against a predefined dataset of the reference spectra, including ferrites metal oxides and organic compounds that aids in the material identification . The FTIR spectra and the labelled peaks along with the calculated parameters are plotted using the plot_ftir( ) where the x-axis represents the wavenumber (inverted as per FTIR) and the y-axis represents absorbance or the transmittance intensity. This visualization ensure a comprehensive evaluation of the spectral features.

5. Conclusion

This study successfully analyzes the characteristics of Co-Zn substituted ferrite by using XRD and FTIR results of these nanomaterials. This study confirms their nanoscale structure and chemical properties. Python based data processing gives an accurate peak detection, crystalline size estimation and functional group identification and other various properties. Future enhancements include AI driven predictive models that can be employed for a better and futuristic approach. These enhancements will contribute to a more efficient, accurate and scalable approach in material characterization analysis.

6. Glossary

- Function – A function in Python is a reusable block of code that performs a specific task, allowing us to avoid repetition by calling it with different inputs instead of rewriting the same code. (e.g. here in our codes identity_peak(), functional_group().
- Polymetallic – Refers to something containing or composed of several metals.
- Ferrimagnetic materials – It exhibit spontaneous magnetization due to the presence of two or more non-identical sublattices with opposing magnetic moments, where the moments do not cancel each other out, resulting in a net magnetization.

5.1 Glossary of FTIR peak analysis

- Absorbance – A measure of how much light is absorbed by a sample at a specific wavenumber.
- Absorption band – A range of wavenumber where a material absorbs infrared light, indicating the presence of certain functional groups.
- Band Gap Energy – The energy difference between the valence and conduction bands in a semiconductor determining its electronic properties.

- Crystallinity – The degree of structural order in a solid, inflecting material properties and spectral peak shapes.
- Full width half maximum (FWHM) – A measure of peak width in a spectrum indicating sharpness or broadening due to material properties.
- Functional group – A specific group of atoms in a molecular responsible for characteristic chemical reaction
- Instrumental resolution - The ability of a spectrometer to distinguish between closely spaced spectral features
- Metal oxides – Compounds containing metal elements bonded to oxygen, often studied for their electronic and catalytic properties
- Molecular interaction – The way molecules interact with each other affecting spectral features such as peak broadening.
- Organic Compounds - Molecules made of carbon and hydrogen often containing functional groups that influence their behavior.
- Peak detection - The process of identifying significant points in spectral data where absorbance or transmittance changes sharply.
- Prominence (of peaks) – A measure of how much a spectral peak stands out form the surrounding baseline, helping in distinguish significant features.
- Semiconductor behavior – A property of materials where electrical conductivity is intermediate between conductors and insulators, influenced by band gap energy
- spectral data - Data representing the intensity of light.
- Transmittance – The fraction of light that passes through a sample without being absorbed.
- Vibrational modes – The ways in which atoms in a molecular more relative to each other, often detected in infrared spectroscopy
- wavenumber (cm^{-1}) - The number of wave cycles per centimeters commonly used in infrared spectroscopy instead of wavelength.

5.2 Glossary of XRD Result analysis

- Crystallographic structure – The arrangement of atoms in a crystalline material determining its physical and chemical properties.
- 2Theta – The diffraction angle measured in degree, representing the angle between incident and diffracted X-rays.
- Intensity – the strength of the diffracted X- rays, indicating how much X-ray radiation is scattered by a material's crystal planes.
- Diffraction pattern – A graphical representation of X- ray intensity versus 2Theta, used to determine material structure
- Bragg's law - A fundamental equation is XRD that relates the wavelength of incident X-ray, interplanar spacing and diffraction angle

- Bragg reflection – The constructive interference of X-rays scattered from different atomic layers forming peaks in XRD spectrum.
- Crystalline size – The size of a single crystal domain in material influencing material properties such as hardness and conductivity.
- Lattice parameters – The physical dimensions of a unit cell in a crystal lattice defining its structure
- Scherrer equation – A formula used to estimate the size of crystallites based on XRD peak broadening.
- Scherrer constant (K) – A dimensionless factor in the Scherrer equation typically around 0.9, depending on the shape of the crystalline
- X-ray wavelength (λ) - The distance between successive wave crests of the X-rays used in diffraction (e.g., Cμ- Kα, 1.5406 Å).
- Full Width at Half Maximum (FWHM, β) – The width of an XRD peak at half of its maximum intensity, used to calculate crystalline size.
- Bragg angle (θ) – Half of the 2Theta value where a diffraction peak occurs, crucial for structural analysis.
- Interplanar spacing (d- spacing) – The distance between parallel crystal planes calculated using Bragg's Law.
- Lattice parameter (a) - The length of the unit cell's edge in a cubic crystal system derived from interplanar spacing and Miller indices.
- Miller indices (h, k, l) – A set of three indices that describe the orientation of the crystal planes in a lattice.
- Phase identification – The process of determining the crystalline phases present in a sample by comparing XRD patterns to reference data.

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