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Raman Spectroscopic Analysis of Barium Zirconate Powder for Investigating Vibrational And Bandgap Energies in Pem Fuel Cell Applications

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ABSTRACT

The project focuses on the synthesis and characterization of $BaZrO_3$ as an advanced ceramic material for PEM Fuel Cell applications. PEMFCs are efficient and eco-friendly power sources but are limited by high catalyst cost and low membrane durability. To overcome these challenges, $BaZrO_3$ was chosen for its excellent chemical stability, thermal resistance, and proton conductivity, making it ideal for enhancing the efficiency and lifespan of fuel cell catalysts. $BaZrO_3$ powder was synthesized using the chemical co-precipitation method, ensuring fine particle size and uniform composition. The process involved reacting barium nitrate and zirconium oxychloride, followed by pH adjustment using sodium hydroxide, drying, and calcination at 1000 °C to obtain crystalline $BaZrO_3$. The material was characterized using X-Ray Diffraction (XRD) and Raman Spectroscopy. XRD confirmed a cubic perovskite structure, while Raman analysis showed vibrations with slight lattice distortions and oxygen vacancies that support ionic transport.

The synthesized $BaZrO_3$ exhibited high thermal and chemical stability, proving its potential as a durable and cost-effective catalyst support for PEM fuel cells. Its strong structural integrity and enhanced ionic conductivity make it a promising material for next-generation clean energy systems with improved efficiency and long-term stability.

Keywords: Energy sources, PEM Fuel cell, Membrane Electrode Assembly, Barium Zirconate, Synthesis, Co-Precipitation method, Physical Characteristics, Raman Spectroscopic analysis, X-Ray Diffraction analysis, Bandgap Energy.

1. INTRODUCTION

Fuel cells are electrochemical devices that convert hydrogen and oxygen directly into electricity through chemical reactions without combustion. They are clean, efficient, and produce mainly water and heat as by-products. A fuel cell consists of an anode, cathode, electrolyte, and catalyst. Hydrogen splits into protons and electrons at the anode, generating electricity, while oxygen combines with them at the cathode to form water. Fuel cells are widely used in vehicles, portable devices, and power systems, with PEM fuel cells being the most popular due to their low operating temperature and quick start-up.

1.1 COMPONENTS OF A FUEL CELL

A fuel cell consists of several important components that work together to produce electricity from hydrogen and oxygen:

1. Anode – The negative electrode where hydrogen is supplied and split into protons and electrons. Electrons flow through an external circuit to generate electricity.
2. Cathode – The positive electrode where oxygen reacts with protons and electrons to form water.
3. Electrolyte – A membrane that allows only ions (protons) to pass through while blocking electrons, enabling electricity generation.
4. Catalyst Layers – Usually made of platinum, these speed up the chemical reactions at the anode and cathode.
5. Bipolar Plates – Distribute gases, collect current, provide structural support, and help manage heat.
6. Gas Diffusion Layers (GDLs) – Ensure uniform gas flow, manage water, and support heat distribution.
7. Membrane Electrode Assembly (MEA) – The core part of the fuel cell containing the membrane, catalyst layers, and GDLs, responsible for the electrochemical reaction.

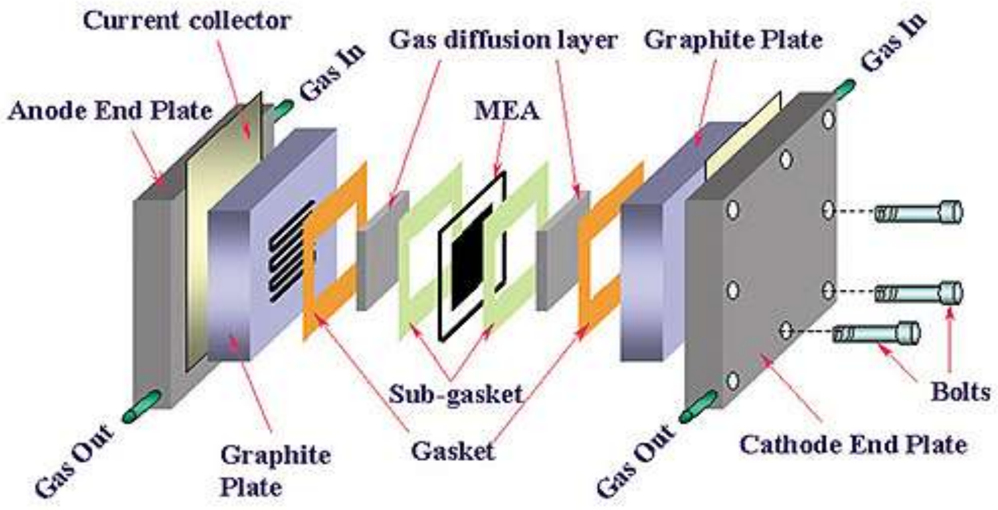

Figure 1.2 Components of PEM fuel cell

1.2 TYPES OF FUEL CELLS

Fuel cells are classified based on the electrolyte used:

- PEM Fuel Cell (PEMFC) – Proton exchange membrane, low temperature
- Solid Oxide Fuel Cell (SOFC) – Ceramic electrolyte, high temperature
- Alkaline Fuel Cell (AFC) – KOH electrolyte
- Phosphoric Acid Fuel Cell (PAFC) – Liquid acid electrolyte
- Molten Carbonate Fuel Cell (MCFC) – Molten carbonate salts

Each type operates at different temperatures and serves unique applications.

1.3 PROTON EXCHANGE MEMBRANE FUEL CELL (PEMFC)

Proton exchange membrane fuel cells (PEMFC) are efficient and versatile fuel cells. Widely used in electronic use It operates at relatively low temperatures (60–80°C) and uses a solid polymer electrolyte membrane to prevent protons from passing through. Electrons and Gas in diffuses to the anode. which are split into protons and electrons via a platinum catalyst. Protons travel across the membrane to the cathode. As the electrons travel through an external circuit (which supplies electricity) to produce electricity, at the cathode, oxygen reacts with incoming protons and electrons to form water. which is the only by-product This clean and efficient operation This, combined with its compact design, makes PEMFCs an attractive option for a wide range of energy.

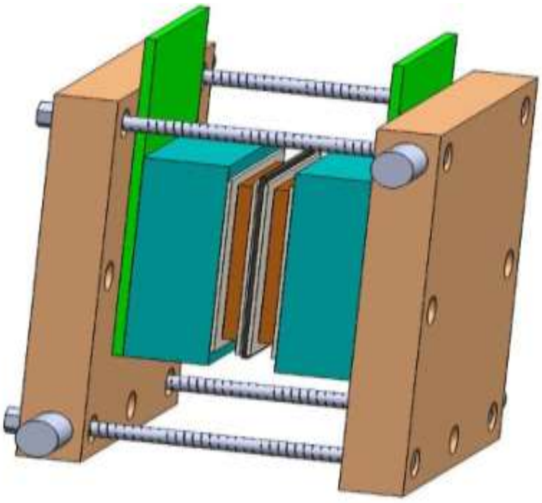

Fig. 1- b- Assembled view of PEM Fuel cell

2. LITERATURE REVIEW

2.1 STUDIES ON PEM FUEL CELL PERFORMANCE

This chapter provides background information on PEM fuel cells through a review of previous studies. Research mainly focuses on improving fuel cell performance, durability, cooling systems, and material selection.

Studies show that the major challenges in PEM fuel cells are poor water management, fuel starvation, corrosion, catalyst poisoning, and temperature control. Improper hydration can cause membrane drying or flooding, reducing efficiency and damaging components (Schmittinger & Vahidi, 2008). Researchers emphasize the need for better thermal and water management systems and durable materials to improve fuel cell lifespan.

Singh et al. (2022) studied the effects of water management and cooling techniques on PEM fuel cell performance. The paper discusses cooling methods such as air cooling, liquid cooling, phase-change cooling, and heat pipes to maintain optimal operating temperature and improve efficiency.

Tabbi et al. (2019) reviewed coating materials and techniques used for bipolar plates in PEM fuel cells. Methods like electroplating, thermal spraying, CVD, and PVD were analyzed for improving corrosion resistance and electrical conductivity while reducing manufacturing cost.

Pramoth Varsan Madhavan et al. (2025) focused on advanced catalyst development for PEM fuel cells. The study highlights low-platinum alloy catalysts and the use of machine learning techniques such as XGB, ANN, and genetic algorithms to predict and optimize catalyst performance for better efficiency and reduced cost.

2.2 STUDIES ON ELECTRODE MATERIALS

Recent studies focus on barium zirconate ($BaZrO_3$ or BZO)-based proton-conducting materials for fuel cells and hydrogen devices due to their high chemical and thermal stability.

Hossain et al. (2021) reviewed BZO proton conductors and explained that doping with trivalent ions such as Y^{3+}, Yb^{3+}, and In^{3+} creates oxygen vacancies that improve proton conductivity. Synthesis methods like solid-state, sol–gel, and co-precipitation strongly affect grain size, densification, and conductivity. Challenges such as grain boundary resistance, poor sinterability, and Ba volatilization were also discussed, along with solutions like co-doping and sintering aids.

Fransson et al. (2023) studied the nanoscale structural behavior of $BaZrO_3$ using molecular dynamics simulations. The study revealed dynamic atomic fluctuations and octahedral tilt instabilities that influence proton transport and defect formation. These findings help explain the material's electrical and structural behavior in fuel-cell applications.

3. PROBLEM IDENTIFICATION AND OBJECTIVES

3.1 PROBLEM IDENTIFICATION

However, their performance is strongly dependent on the properties of electrolyte and electrode materials, particularly their ionic conductivity, chemical stability and compatibility with the membrane traditional materials such as Nafion or membranes exhibit limited thermal stability and high cost, making the search for alternative ceramic proton conductors essential.

Barium Zirconate ($BaZrO_3$), a perovskite-type oxide, is known for its excellent chemical stability, high proton conductivity, and wide bandgap. However, the correlation between its structural vibrations and electronic band structure is not well understood. A detailed Raman spectroscopic study is necessary to identify vibrational modes, defect structures, and bandgap characteristics, which directly influence the ionic conduction and electrochemical performance of $BaZrO_3$ in fuel cell environments.

Hence, the problem lies in the lack of comprehensive spectroscopic understanding of $BaZrO_3$ powder prepared via co-precipitation method, which affects its optimization for PEM fuel cell applications.

3.2 OBJECTIVES

- To perform Raman spectroscopic analysis for identifying vibrational modes associated with the perovskite $BaZrO_3$ structure.
- To investigate the relationship between vibrational characteristics and defect formation, which influences proton conductivity.
- To estimate the bandgap energy of $BaZrO_3$ using spectroscopic data and correlate it with its suitability for PEM fuel cell operation.

4. MATERIAL SELECTION AND SYNTHESIS METHOD

4.1 BARIUM ZIRCONATE ($BaZrO_3$)

Barium Zirconate ($BaZrO_3$) is a perovskite ceramic material known for its excellent chemical stability, thermal resistance, and ionic conductivity. In this project, it is used as a coating material for platinum catalysts in PEM fuel cells to improve performance and durability. $BaZrO_3$ protects the catalyst from degradation, agglomeration, and sintering during operation. It also supports better proton conductivity, maintains high electrochemically active surface area (ECSA), and performs well in acidic environments. Compared to materials like CeO_2, $BaZrO_3$ offers better long-term stability and helps reduce platinum usage, improving fuel cell efficiency and lifespan.

4.2 PROPERTIES OF $BaZrO_3$

$BaZrO_3$ has several important properties:

- Chemical Formula: $BaZrO_3$
- Density: 6.25 g/cm^3
- Melting Point: ~2570°C
- Insoluble in water
- High thermal stability and chemical resistance
- Good ionic and electrical conductivity at high temperatures
- Stable dielectric properties
- Good compatibility with catalysts
- Compared with TiO_2, ZrO_2, and CeO_2, $BaZrO_3$ provides a balanced combination of high thermal stability, excellent chemical resistance, and good ionic conductivity, making it highly suitable for advanced fuel cell applications.

4.3 MATERIAL SYNTHESIS PROCESS

$BaZrO_3$ powder was synthesized using the co-precipitation method. Barium nitrate and zirconium oxychloride were dissolved in distilled water and stirred at 60 °C for uniform mixing. Sodium hydroxide (NaOH) was added dropwise to adjust the pH to 10, causing precipitation of metal hydroxides. The precipitate was aged, filtered, washed with water and ethanol, and dried at 80 °C for 12 hours. Finally, the powder was calcined/annealed in a muffle furnace at 500–1000 °C for 4 hours to obtain crystalline $BaZrO_3$ powder.

4.4 CO-PRECIPITATION METHODOLOGY

In the co-precipitation method, Ba and Zr precursor solutions react in an alkaline medium to form $BaZrO_3$ precipitate. The product is then heated, washed, filtered, dried, and annealed to achieve pure and uniformly distributed $BaZrO_3$ powder with good crystallinity and phase purity.

Figure: 4.1 Co Precipitation Methodology

4.5 MATERIAL SAMPLE

The $BaZrO_3$ powder sample presented in figure 4.2 appears to exhibit the characteristic fine, uniformly distributed morphology typical of perovskite-type ceramic materials synthesized through co-precipitation method.

Figure: 4.2 $BaZrO_3$ Powder

5. CHARACTERIZATION TECHNIQUES

5.1 PHYSICAL CHARACTERIZATION TECHNIQUES

Physical characterization techniques are used to study the phase formation, crystallinity, particle size, and surface properties of materials, which are important for improving PEM fuel cell performance.

5.2 X-RAY DIFFRACTION (XRD) ANALYSIS

XRD is an important technique used to identify crystal structure, phase purity, lattice parameters, and crystallite size of materials. In this study, XRD analysis of $BaZrO_3$ was carried out using a Rigaku MiniFlex diffractometer with Cu Kα radiation over a 2θ range of 10°–80°.

Figure 5.1 Experimental setup of X-ray diffraction analysis

The analysis is based on Bragg's Law:

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

This equation helps calculate interplanar spacing (d-spacing) and identify crystal planes.

Where n is the order of diffraction (typically taken as 1), λ is the wavelength of the incident X-rays, d is the interplanar spacing, and θ is the Bragg diffraction angle corresponding to each peak in the XRD pattern of the crystal plane.

The crystallite size was estimated using the Scherrer equation:

$$D = \frac{K\lambda}{\beta\cos\theta}$$

In this relation, D represents the approximate size of the crystalline domains, which may match or be smaller than the actual grain size and is usually reported in nanometers. The factor K is a unitless shape constant and is generally assumed to be about 0.9. The symbol λ corresponds to the wavelength of the X-ray used (1.54 Å), while β refers to the peak's Full Width at Half Maximum (FWHM). The angle θ simply indicates the diffraction angle measured during the analysis.

XRD results confirmed the formation of crystalline perovskite $BaZrO_3$, detected impurity phases, and showed the nanocrystalline nature of the material. These properties are important for proton conductivity and fuel cell applications.

5.3 RAMAN SPECTROSCOPY

Raman spectroscopy is used along with XRD to study the structural and chemical properties of materials. Unlike XRD, which analyzes crystal structure, Raman spectroscopy provides information about molecular vibrations, chemical bonds, and structural changes.

In this technique, a laser beam is directed onto the sample, and the scattered light produces characteristic Raman peaks that help identify bonding environments, crystallinity, carbon phases, and metal-support interactions in catalyst materials.

Raman spectroscopy is especially useful for detecting amorphous phases and structural defects that may not appear in XRD analysis. However, issues such as fluorescence, weak signals, and laser heating can affect the results. Combined with XRD, Raman spectroscopy provides a more complete understanding of the catalyst structure and synthesis quality.

5.4 BAND GAP ENERGY ANALYSIS

The band gap energy of $BaZrO_3$ is influenced by its crystal structure and bonding characteristics, which are analyzed using XRD and Raman spectroscopy.

XRD confirms the cubic perovskite structure, lattice parameters, and structural strain, all of which affect the electronic band structure and band gap energy.

Raman spectroscopy provides information about local bonding, oxygen vacancies, and lattice distortions. In ideal cubic $BaZrO_3$, Raman activity is weak, so the presence of Raman peaks indicates structural defects or symmetry changes.

Sharp Raman peaks indicate strong and ordered Zr–O bonds with a wider band gap, while broadened peaks suggest defects or disorder that can reduce the band gap slightly. Together, XRD and Raman analysis help understand the structural and electronic properties of $BaZrO_3$.

6. RESULTS AND DISCUSSION

6.1 X-RAY DIFFRACTION (XRD) ANALYSIS

The XRD analysis confirms that the synthesized $BaZrO_3$ has successfully formed a high-purity, single-phase cubic perovskite structure. The diffraction peaks at specific 2θ values match the standard planes of $BaZrO_3$, indicating a $Pm\bar{3}m$ cubic structure with no impurity phases such as $BaCO_3$ or ZrO_2.

Peak broadening suggests that the material is nanocrystalline, with crystallite size estimated in the range of 20–40 nm using the Scherrer equation:

$$D = \frac{K\lambda}{\beta\cos\,\theta}$$

The calculated lattice parameter is close to the standard value (~4.19 Å), confirming good structural formation with slight deviations due to strain or oxygen vacancies.

Overall, XRD results show that $BaZrO_3$ has a well-defined cubic structure with nanocrystalline nature, and minor lattice distortions that may enhance its electrochemical properties for PEM fuel cell applications.

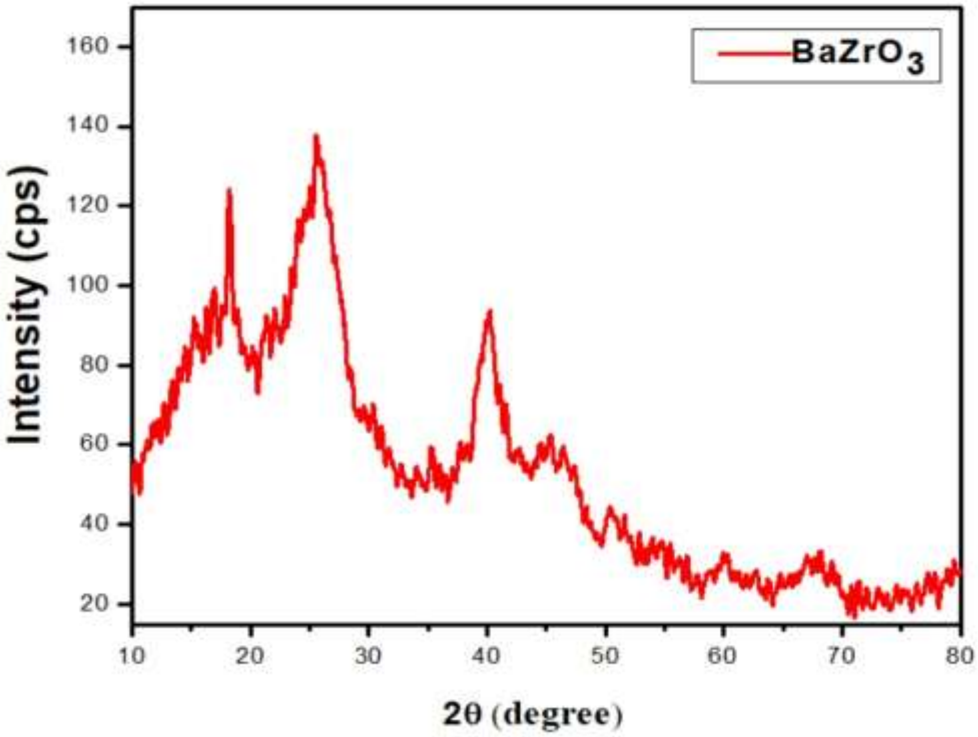

Figure 6.1 XRD Pattern of $BaZrO_3$

6.2 RAMAN SPECTROSCOPY ANALYSIS

Raman spectroscopy was used to study the vibrational and structural properties of $BaZrO_3$. Since cubic $BaZrO_3$ is mostly Raman-inactive, the spectra show broad, weak, and diffuse features rather than sharp peaks, confirming a highly ordered cubic perovskite structure.

The observed signals mainly arise from second-order and multi-phonon scattering related to Zr–O lattice vibrations. No impurity peaks (such as $BaCO_3$ or ZrO_2) were detected, confirming high phase purity of the sample.

Both Raman spectra (200–1800 cm⁻¹) indicate minimal structural distortion, with slight broad features attributed to oxygen vacancies, lattice strain, and nanocrystalline effects. These features suggest local disorder within an overall cubic structure, which can influence ionic and proton transport properties.

Overall, Raman results support the XRD findings, confirming that the synthesized $BaZrO_3$ is a pure, well-ordered cubic perovskite suitable for fuel cell applications.

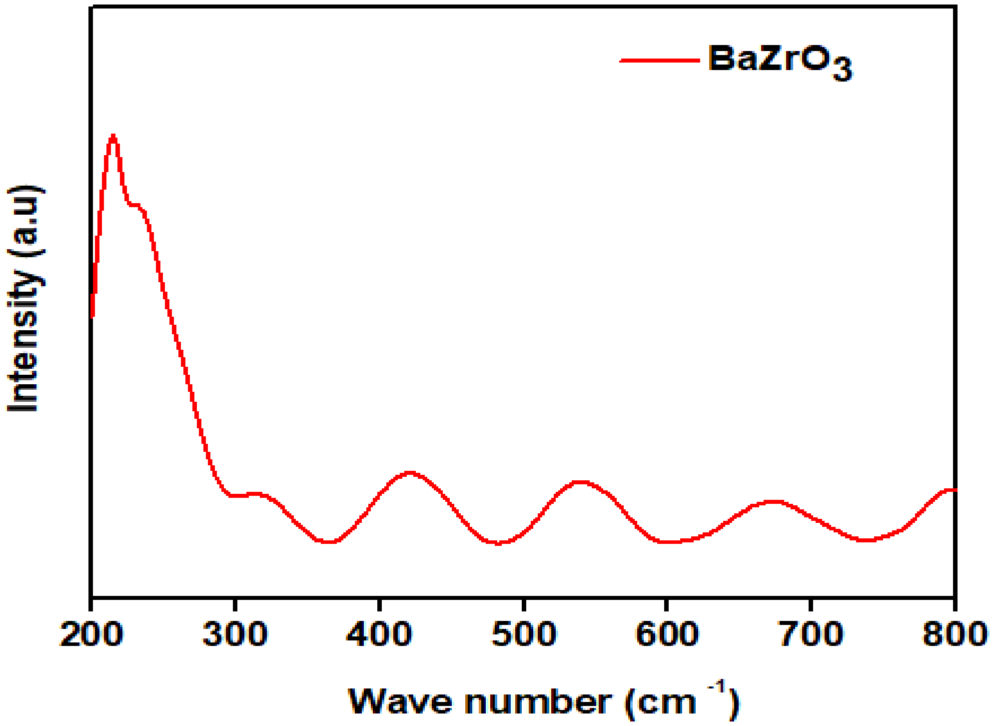

Figure 6.2 Raman Spectra of $BaZrO_3$

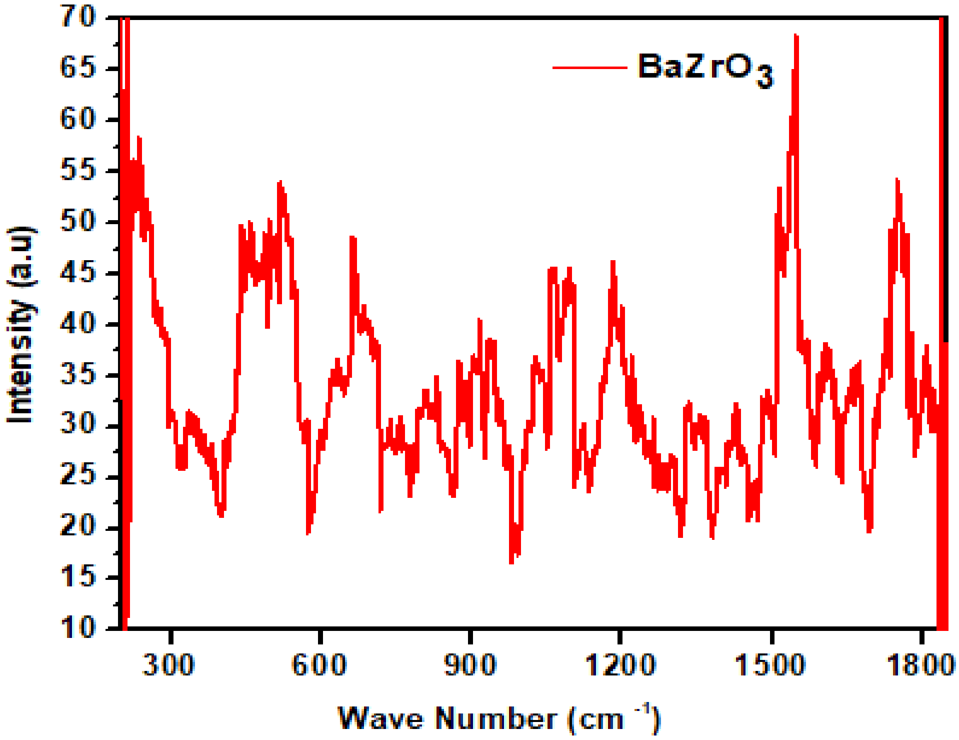

Figure 6.3 Raman Spectrum of $BaZrO_3$

6.3 BAND GAP ENERGY ANALYSIS

The band gap energy of $BaZrO_3$ is influenced by its crystal structure, lattice strain, and oxygen vacancies, as confirmed by XRD and Raman analysis.

XRD results show a cubic perovskite structure with nanocrystalline features, peak broadening, and slight lattice distortions, indicating the presence of defects and oxygen vacancies. Raman spectroscopy supports this by showing broad, weak second-order vibrational features typical of a highly symmetric cubic structure with minor local disorder.

These structural defects introduce localized energy states near the band edges, which can slightly modify and generally reduce the band gap compared to an ideal structure. Overall, the combined XRD and Raman results show that the electronic properties of $BaZrO_3$ are strongly linked to its microstructure, making it important for proton-conducting and electrochemical applications.

7. CONCLUSION

The synthesized $BaZrO_3$ powder was successfully characterized using XRD and Raman spectroscopy, confirming its high purity and stable cubic perovskite structure. XRD results showed a single-phase material with good crystallinity and appropriate lattice parameters, indicating structural stability suitable for PEM fuel cell applications.

Raman analysis supported these findings by showing broad, weak vibrational features typical of cubic $BaZrO_3$, with no impurity peaks, confirming chemical purity and minimal lattice distortion.

Overall, the combined XRD, Raman, and band gap analyses confirm that the prepared $BaZrO_3$ has excellent structural quality, stability, and properties suitable for use in PEM fuel cells and other electrochemical applications.

8. ACKNOWLEDGEMENT

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