GREEN SYNTHESIS OF $BaFeO_3$ PEROVSKITE USING CITRUS LIMON EXTRACT

B. Breezy, C. Infant Francita Fonseka

Department of Physics, St. Mary's College (Autonomous), Thoothukudi,
Affiliated to Manonmaniam Sundaranar University, Tirunelveli, Tamil Nadu, India

ABSTRACT:

This study reports the green synthesis of BaFeO3 perovskite using Citrus limon extract as a reducing agent. The structural, optical, and morphological properties of the synthesized material were analyzed using X-ray diffraction (XRD) and ultraviolet-visible spectroscopy (UV-Vis). The XRD pattern confirmed the formation of the BaFeO3 perovskite phase with the crystallite size to be 9.49 nm, while the UV-Vis spectrum showed a bandgap energy of approximately 1.348 eV. The results of this study demonstrate the potential of green synthesis methods for the production of functional materials, while also highlighting the promise of BaFeO3 perovskite.

KEYWORDS: $BaFeO_3$, perovskite, supercapacitor, XRD, UV, nanoparticles

INTROUCTION:

Nanotechnology represents a revolutionary path for technological development that concerns the management of materials at the nanometer scale. Nano-fabrication is a natural step toward further reducing the physical size of the components and functional parts to provide a variety of applications [1]. Unique electrical properties, such as high conductivity in materials like carbon nanotubes and graphene. Perovskite refers to a class of materials with a specific crystal structure. Nanomaterial-based supercapacitors are used to increase the electrode surface area so as to achieve high performance and enhanced capacitance [2].

OBJECTIVE OF THE PRESENT WORK:

- To synthesize $BaFeO_3$ perovskite material using the fresh juice of citrus limon through green synthesis.
- To find the crystalline size and phase of $BaFeO_3$ perovskite using XRD.
- To find the optical characteristics of $BaFeO_3$ perovskite to be employed in opto-electronic field using UV.

MATERIALS AND METHODOLOGY:

Ba $(NO_3)_2$ is an inorganic compound with chemical name Barium nitrate. It is a good oxidizing agent, burns with a green coloured flame. It is a non-combustible compound, but enhances the burning of combustible elements. When exposed to fire or heat for a long duration it may explode. Ferric nitrate is also referred to as Iron (III) nitrate or iron trinitrate, whose chemical or molecular formula is $Fe(NO_3)_3$ or FeN_3O_9. It is a strong oxidant and non-combustible chemical compound. Though it is non-flammable, it will increase the intensity of a fire if it comes in contact with combustible materials. Citrus limon is a bright yellow citrus fruit. Lemon juice is a rich source of citric acid, containing around 48 grams per liter. It is a weak organic acid naturally found in citrus fruits. Citric acid acts as a preservative, antioxidant and adds acidity, while also altering the pH and enhancing mineral absorption.

EXPERIMENTAL PROCEURE:

The preparation of $BaFeO_3$ was done by sol-gel process. 5.23 g of $Ba(NO_3)_2$ and 8.07 g of $Fe(NO_3)_2.9H_2O$ was measured and added to a beaker along with 150 ml of deionized water and 50 ml of fresh juice of citrus limon was added. This mixture was placed in a magnetic stirrer and heated. 45 ml of Ethylene glycol was added as a complexing agent. The mixture was heated until completely evaporated forming a dry brown precipitate. This precipitate was placed in the muffle furnace for 4 hours at 600 °C and the resultant was crushed finely with the help of a motor and pestle, thus obtaining a reddish brown sample. Further, $BaFeO_3$ was sent for various analysis.

Figure 1: Precipitate before and after calcination

X-RAY DIFFRACTION:

X-ray diffraction (XRD) is a versatile non-destructive analytical technique used to analyze physical properties such as phase composition, crystal structure and orientation of powder, solid, liquid samples and even dispersed particles in a liquid matrix. Sample preparation is minimal and is suitable for use both in industrial process applications and in materials research.

The Debye-Scherrer method is a technique that uses X-ray diffraction to analyze the crystalline structure of a powder sample, forming Debye-Scherrer rings, which can be used to determine lattice spacing and estimate particle size.

UV-VIS SPECROSCOPY:

UV-Vis spectroscopy is an analytical method that can measure the analyte quantity depending on the amount of light received by the analyte. Applicable for both organic and inorganic samples. As a function of wavelength, UV-vis spectrophotometers measure the absorption or transmission of light that passes through a medium. According to the Beer-Lambert Law, the absorbance is directly proportional to the concentration of the substance in the solution.

RESULTS AND DISCUSSTIONS:

CHARACTERIZATION USING XRD:

The structural characterization of the synthesized material $BaFeO_3$ is carried out by the XRD method. The X-ray diffraction experiments are carried out at wavelength 1.5406 A°. Peak in the pattern corresponds to constructive interference of X-ray of X-rays from the

specific crystallographic planes.

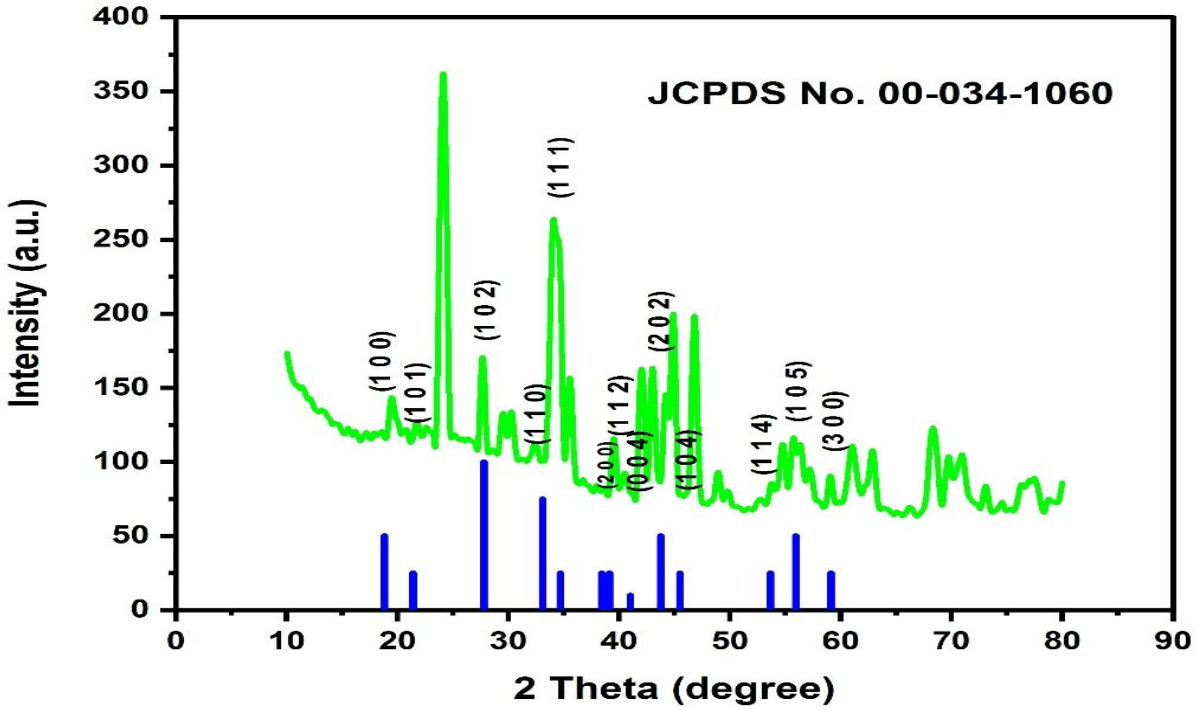

Figure 2: XRD pattern for $BaFeO_3$ perovskite

The average grain size is calculated using the Debye Scherrer formula, $D = \frac{K\lambda}{\beta \cos\theta}$ (nm)

K - Shape factor (approximately 0.9)

β - Full width at half maximum (FWHM) of a diffraction peak

λ - X-ray wavelength

θ - Bragg angle

The XRD results for the $BaFeO_3$ perovskite nanoparticles, by Debye Scherrer equation is found to be 9.49407 nm. The XRD results for the $BaFeO_3$ exhibit strong peaks around 24.587°.

Crystal system	Hexagonal
Crystalline size (nm)	9.49
Lattice parameter a(A°)	5.4090
Lattice parameter b(B°)	5.4090
Lattice parameter c(C°)	8.7950
Volume of the unit cell	222.84

CHARACTERIZATION USING UV-Visible Absorption Spectra of $BaFeO_3$ Nanoparticles:

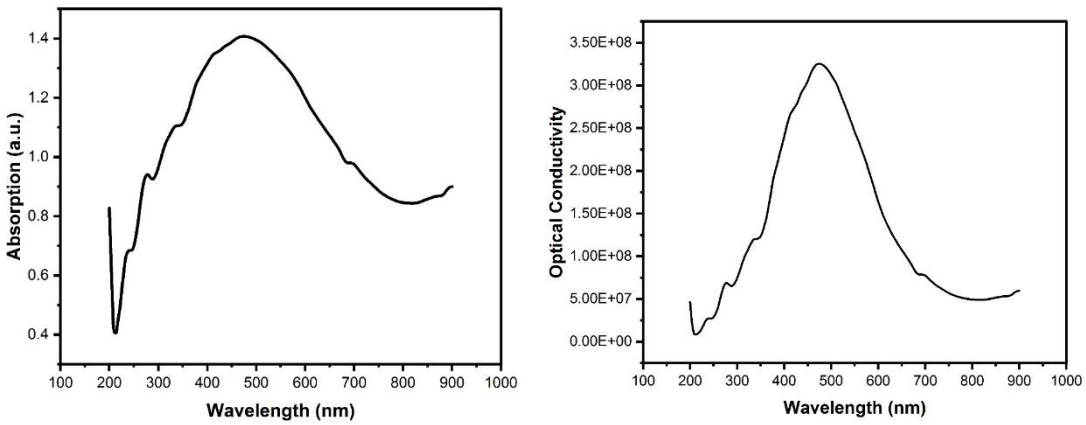

Figure 3: Absorption and optical conductivity of $BaFeO_3$

The absorption is relatively low near 300 nm (UV) and reaches a maximum peak around the range 400–500 nm, indicating a strong absorption of light in this region. After this region, the adsorption gradually decreases. Moreover there is a dip in absorption around 300-350 nm before reaching the peak. The peak 400-450 nm range shows that the sample absorbs visible light, hence could find its application in photodetectors and optoelectronics devices.

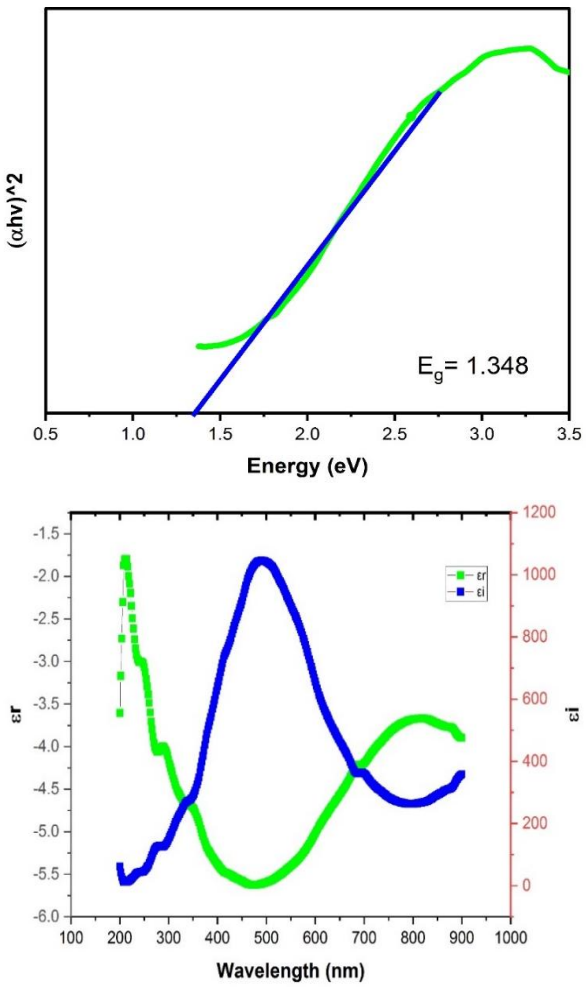

Figure 4: Energy bandgap and dielectric constant of $BaFeO_3$

The optical conductivity increases as the wavelength is 100 nm, reaching a broad maximum peak around 400 to 500 nm. After reaching its peak, the optical conductivity decreases as the wavelength increases beyond 550 nm. The peak indicates more absorption around 400-550 nm and hence conducts the most electrical current due to photo-generated carriers. The observe peaks and valleys in the graph related to electronic transitions between different energy bands in the material. Due to high optical conductivity in the visible light region, $BaFeO_3$ can be employed in solar cells and other devices that requires visible light absorption.

The graph represented is a Tauc plot utilized for determining the energy bandgap and this method is important for analyzing the electronic properties of a semiconductor material. The bandgap is identified by extrapolating the linear portion to the x-axis. In this case the value is E_g=1.348 eV.

This graph presents the dielectric properties of the synthesize material, $BaFeO_3$, with εr as the real and εi as the imaginary plot. Real part: Represents the material's ability to store

electrical energy. There is a sharp increase in value near 400 nm, then 400-700 nm shows variability and beyond 700 nm εr stabilizes and decreases gradually. Imaginary part: This part of the graph represents the material's dielectric loss, which is dissipated as heat. Near 320-450 nm there is a significant peak indicating high energy loss and from 450 to 900 nm there is a gradual decrease with minor fluctuations.

CONCLUSION:

This study focused on the synthesis and characterization of $BaFeO_3$, a perovskite material as a potential electrode material. Green synthesis of the material was carried out with citrus limon to promote an eco-friendly move in energy application.

The XRD characterization revealed that the crystalline nature of the prepared $BaFeO_3$ is hexagonal structure. The average particle size is found to be 9.494 nm. From the UV analysis the energy bandgap is found to be 1.348 eV and shows good absorbance.

REFERENCE:

1. Jayaprakash Meena, Shapna Shankari Sivasubramanian, Ezhumalai David, Santhakumar K (2024), Green supercapacitors: review and perspectives on sustainable template-free synthesis of metal and metal oxide nanoparticles, From the journal of: RSC Sustainability volume 2, pp 1224-1245.
2. Ashna K. Pramod and Sudip K. Batabyal (2024), *Perovskite Photodetector*, From the journal: Perovskite Optoelectronic devices, pp 397-416.
3. Y. Sakout, O. El Ghadraoui, E.H. Lahrar, M. Zouhairi, N. Tijani, A.Harrach and T. Lamcharfi (2024), Synthesis, Structural and Morphological Characterization and Dielectrical Behavior of $BaFeO_3$-x, From the journal: Integrated ferroelectrics, Volume 240, Issue 1.
4. G. Jayanthi, Sowrirajan Sumathi, Karthik Kannan, V. Andal, Sivaraj Murugan (2022), A review on the synthesis, properties and environmental application of Fe- Based Perovskite, From the journal: Advances in material sciences an Engineering, Issue 1/6607683.