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EFFECT OF SHOCK WAVES ON BISMUTH FERRITE OXIDE (BFO) NANOPARTICLES SYNTHESIZED BY HYDROTHERMAL METHOD

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Abstract

Bismuth ferrite oxide nanoparticles (BFO NPs) are a promising material due to their multifunctional properties, including magnetoelectric, photocatalytic, and energy storage capabilities. This study explores the impact of mechanical shock loading on the structural, vibrational, morphological, and optical properties of $BiFeO_3$ nanoparticles. The Bismuth ferrite oxide nanoparticles are synthesized via the hydrothermal route. Characterization techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and UV-Vis absorption spectroscopy were employed to assess the changes in the structural and optical properties caused by the shock pulses. XRD analysis revealed that the shock treatment-induced slight changes in the crystallinity and lattice parameters of the nanoparticles, with the formation of small strains within the perovskite structure. FTIR spectra indicated that the vibrational modes associated with the Bi-O and Fe-O bonds were slightly shifted after shock loading, signifying modifications in bond strength. SEM analysis showed that while the particle size of the shock-loaded nanoparticles remained in the nanoscale range, there was a noticeable change in morphology, with a more compact and agglomerated structure related to shocked nanoparticles. UV-Vis's spectroscopy demonstrated Bandgap (Eg) for BFO nanoparticles was found to be 3.23 eV and for shock-loaded BFO nanoparticles 3.29 eV.

Keywords: Bismuth ferrite oxide nanoparticles (BFO NPs), Phase transitions, shock-loading.

1 Introduction

In recent years, we observed a great deal of work done by materials scientists and device engineers to create effective materials for device applications in ambient and non-ambient situations [1]. The structure-property relationship against high pressure and high temperature is a trivial requirement for applications using ambient conditions [2]. However, we need to be conscious of the structure-property link in aircraft, thermal protection systems, and military applications where high pressure and high temperature are present [3]. Most materials exhibit significant changes in their chemical and physical characteristics when exposed to high temperatures and pressures [4]. Hence, selecting the best materials for effective applications requires a thorough understanding of the materials' structural, thermal, optical, electrical, and magnetic capabilities under extremely high pressure and temperature circumstances [5].

One effective method for identifying materials that can withstand high temperatures and pressures for device applications is shock waves [6]. Because shock waves simultaneously produce high pressure, temperature, tension, and dynamic impact, among other effects. However, we can adjust the properties with or without altering the original crystal system by employing modest shock waves. Furthermore, from the perspective of applied physics and materials research, these tests pave the way

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for a thorough understanding of the material properties. As a result, the shock wave recovery test offers several benefits over metals, metal oxides, organic and inorganic bulk, and nanocrystalline materials discovered that some of these materials undergo phase transitions, and others are capable of structural deformations in addition to thermal, magnetic, and optical characteristics [7]. Bismuth ferrite (BFO) is an attractive multifunctional material that unites ferroelectric and magnetic properties at room temperature [8].

In bulk form, BFO manifests a perovskite structure with high ferroelectric polarization and antiferromagnetic ordering, which has led to significant interest in memory devices, sensors, and actuator applications [9]. However, when reduced to the nanoscale, $BiFeO_3$ exhibits enhanced properties associated with its bulk counterparts, such as increased surface area, modified crystal structure, and improved electronic, optical, and magnetic behavior [10]. Nanostructured BFO, in the form of nanoparticles, shows promise in various fields due to its size-dependent properties [11]. The reduction in particle size increases the surface-to-volume ratio, which can influence the material's electrical, magnetic, and catalytic performance. These unique characteristics make BFO nanoparticles ideal for a wide range of applications, including energy storage, environmental cleanup, piezoelectric nanogenerators, and spintronic devices [12].

The synthesis of BFO nanoparticles can be achieved through various methods, such as sol-gel, co-precipitation, hydrothermal, solvothermal, sonication, and ball milling techniques. Each has its advantages in terms of particle size control and crystallinity [13]. However, obstacles such as sustaining structural stability, controlling particle size and distribution, and scaling up the synthesis processes need to be addressed to optimize and realize the potential of BFO nanoparticles [14, 15].

In this paper, BFO nanoparticles are synthesized by hydrothermal method and subjected to shock-loaded conditions. Further, various characterization techniques such as Powder XRD analysis, UV-visible spectroscopy, FTIR analysis, scanning electron microscopy, and EDX analysis.

2. Materials and methods

2.1 Materials

All the Chemicals used in this work were analytical grade reagents (AR) Bismuth (III) nitrate pentahydrate (Bi (NO3)3.5H2O), Ferric Nitrate (Fe (NO3)3.9H2O), Citric acid monohydrate (C6H8O7.H2O) and Ammonia solution (NH4OH) were used as starting material with a high purity of (99.9%) without further purification were purchased from Merck company. Double distilled water was used to prepare all solutions.

2.2 Synthesis of BFO nanoparticles and shock-loaded BFO Nanoparticles

For the synthesis of BFO nanoparticles using the hydrothermal method 0.1M of Bismuth (III) nitrate pentahydrate and Ferric Nitrate were dissolved in a beaker filled with 50ml of double distilled water added to that and stirred well using magnetic stirring at room temperature for about 30mins. 0.2M of Citric acid was added equally to the present total molar amount of metal nitrate in the solution. Then the above mixture of the solution was well stirred for about 2 hours at room temperature followed by the ammonia solution was slowly added dropwise to adjust the pH value at 9 to maintain the solution. Continuously the stirring process continued for about 2 hours at room temperature. The final mixture was transferred into a Teflon-lined stainless-steel autoclave with a capacity of about 70 ml. The autoclave was sealed well and heated closed at 180 °C for around 20 hours. Then it is cooled at room temperature after the precipitate was collected. Followed by several times it is washed with deionized water and anhydrous ethanol. After that, it is dried in air at 120 °C for 5 hours. Then calcinated at 600 °C for 5 hours. At last, the bismuth ferrite powder was obtained.

3. Results and Discussion

The synthesized BFO and shock-loaded BFO nanoparticle samples were characterized using powder XRD crystalline analysis, Scanning Electron Microscopy

(SEM) morphological analysis, Fourier transform infrared (FTIR) spectral analysis, and UV-Vis spectral analysis.

3.1 Powder X-Ray Diffraction Analysis.

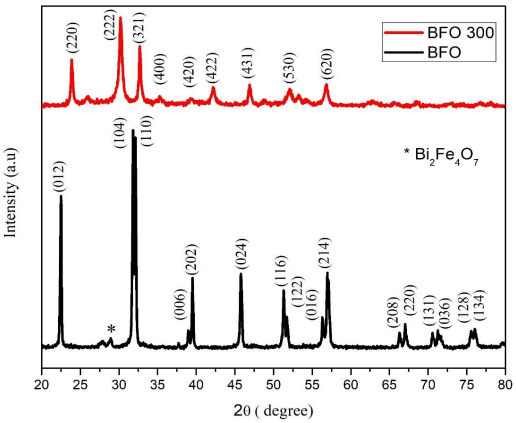

Fig. 1: shows the XRD pattern of control and shock-loaded BFO nanoparticles

The XRD pattern of the bismuth ferrite sample annealed at 600̊ C indicates the pure phase with rhombohedral perovskite structure of bismuth ferrite. The diffraction peaks are very intense and sharp, suggesting the good crystallite nature of the nanoparticles. The JCPDS card no.71-2494 of pure BiFeO3 shows that diffraction from the planes (012), (104), (110), (006), (202), (024), (116), (122), (016), (214), (208) and (220) for the formation of a pure phase of bismuth ferrite. Some traces of impurity phases of Bi2Fe4O7 are also observed in the XRD pattern due to the kinematics of the reaction. The 300 shock-loaded sample becomes broad and shifts to lower 2θ values.

The JCPDS card: 46-0416 of Bi25FeO40 shows that the diffraction from the planes (110), (220), (222), (321), (400), (420), (422), (431), (530), (620) for the formation of Bi25FeO40 with cubic body-centered structure. This indicated that the phase transition has occurred from Rhombohedral with the rhomb-centered to cubic with body-centered. The average crystallite size is calculated based on the Scherrer formula and found to be 45 nm and 21 nm for pure and shock-loaded samples.[19]

3.2 UV-Vis Spectral analysis

The UV–is absorbance range of pure and shock pulsed samples are shown above in Fig.3. The charge transfer of Bi-O is situated at around 250 nm and 360 nm, in addition to that the peak is around 490 nm as a cause of the Fe-O charge transfer band. The strong band observed in the wavelength range of 400-600 nm is attributed to metal-metal transition and the weak band around 700 nm is assigned to crystal field transition.

The band gap is calculated using the given relation

Eg=hc/λ (eV)

The band gap for BiFeO3 nanoparticles was found to be 3.23 eV and for shock-loaded BiFeO3 nanoparticles 3.29 eV. While comparing the absorption spectra of control and shock wave-loaded BiFeO3 nanoparticles, a blue shift in the controlled sample has been shifted to the red region in the shock wave-loaded BiFeO3 nanoparticles.

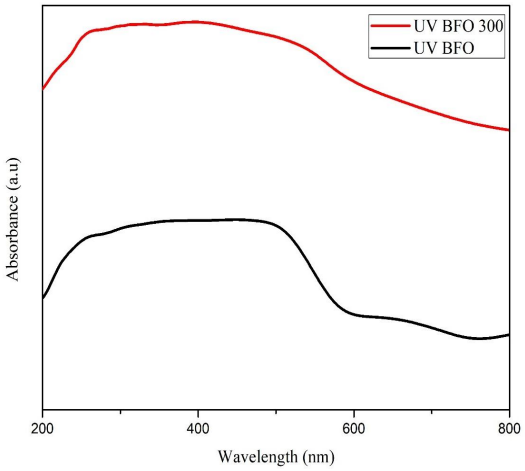

Fig. 2: shows UV-vis spectra of BFO and shock-loaded BFO Nanoparticles

3.3 FTIR Analysis

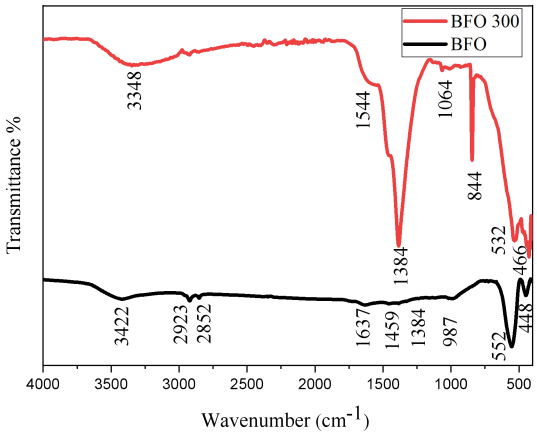

Fig. 3: presents the FTIR spectrum of control and shock-loaded BFO NPs

Fig. 2 shows the FTIR spectrum of pure and shock-loaded Bismuth ferrite nanoparticles. The absorption bands at 3422 cm-1 and 1637 cm-1 are attributed to OH stretching and bending vibration of water molecules. The peaks at 2923 cm-1 and 2852 cm-1 are due to C-H stretching with a narrow band. The peaks at 1384 cm-1 and 1487 cm-1 are due to C-H symmetric and asymmetric bending vibrations. The peaks at the positions of 552 cm-1 and 448 cm-1 are due to the stretching and bending vibrations of the Fe-O. Due to the high crystalline phase, pure BFO has a Bi-O vibration peak at 987 cm-1. For shock-loaded BFO the peaks exist from 400 to 700 cm-1 due to the existence of metal oxides. The Fe-O stretching and bending vibration are responsible for the large peaks at 448 cm-1 and 532 cm-1. The metal-oxygen band of Fe-O, which constitutes around 844 cm-1 range related to the emergence of high-crystalline BFO. The absorption peak at 1064 cm-1 is attributed to the C-O bond. The presence of the carbonyl group confirms the existence of bio-organic compounds in the synthesized sample. The presence of traces of trapped nitrates group at the peak 1384 cm-1. The absorption peak at 1544 cm-1 results from the bending vibration of water molecules absorbed from the atmosphere [16],[17],[18].

3.4 Morphological analysis

The SEM images of control and shock wave-loaded BFO nanoparticles are shown in Fig 4 (a) and 4(b). From the typical SEM image of a control sample, it is observed that uniform spherical BFO nanoparticles were formed with less agglomeration. For the shock wave-loaded sample, a porous-like structure and traces of a secondary phase are noticed. It is also seen that there is a high interconnection of grains with regular, dense, porous, and uniform morphology of BFO nanoparticles.

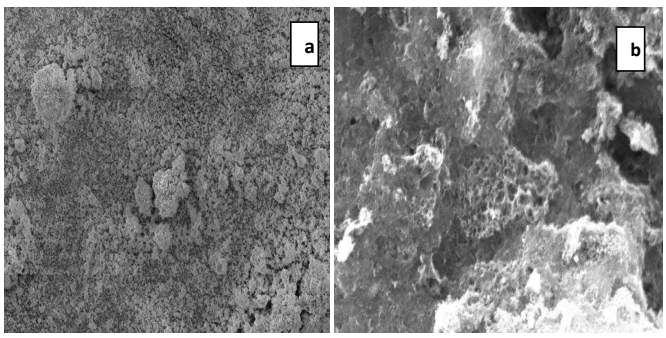

Fig. 4: SEM images of control and Shock wave-loaded BFO nanoparticles

Conclusion

The control and shock-loaded BFO nanoparticles were synthesized using the hydrothermal method. The crystallite nature of synthesized samples is determined using Powder X-ray Diffraction analysis. The crystallite size of the particles is identified using Debye-Scherrer's method which is about 45nm for BFO and 21nm for shock-loaded given nanoparticles respectively. The presence of functional groups was confirmed using FTIR interpretation. The band gaps of synthesized samples were studied using UV-Vis's analysis is 3.23 eV and 3.29 eV for pure and shock-loaded nanoparticles respectively. The surface morphology was determined using SEM analysis.

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