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Analysis of piezoelectric properties of barium titanate ($BaTiO_3$) using ANSYS APDL: a specialized study in electromechanical engineering

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Barium titanate is an important ceramic material in piezoelectric devices. Barium titanate (BT) was prepared via a hydrothermal process at 200 °C for 24 hours. This study initially focused on characterizing barium titanate nanoparticles ($BaTiO_3$) by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) was used to determine the crystalline structure of the material and the functional groups present in the sample. Additionally, the structure and composition of $BaTiO_3$ were confirmed using an energy dispersive spectroscopy (EDS). A disk of barium titanite was made and sintered at a temperature of 1000°C for 4 hours. To simulate the material to confirm its piezoelectric properties, the density was measured and impedance spectra were studied to determine the relative and absolute permittivity; this data was then entered into APDL ANSYS program. The complexity of the resonant modes present in the material causes a piezoelectric response with multiple peaks over a wide frequency range. These peaks can be used to study situations where a specific frequency response of the material is required.
Keyword: hydrothermal, barium titanate, APDL ANSYS, piezoelectric properties, resonant.

Аналіз п’єзоелектричних властивостей титанату барію ($BaTiO_3$) за допомогою ANSYS APDL: Спеціалізоване дослідження в галузі електромеханічної інженерії.
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Титаніт барію є важливим керамічним матеріалом для п’єзоелектричних застосувань. Титанат барію (BT) був отриманий за допомогою гідротермального процесу при 200 °C протягом 24 годин. Це дослідження спочатку було зосереджено на характеристиках наночастинок титанату барію ($BaTiO_3$) за допомогою рентгенівської дифракції (XRD). Інфрачервона спектроскопія з перетворенням Фур’є (FTIR) використовувалася для визначення кристалічної структури матеріалу та функціональних груп, присутніх у зразку. Крім того, структура, а також склад $BaTiO_3$ були підтверджені за допомогою енергодисперсійної спектроскопії (EDS). Був виготовлений диск з титаніту барію, який спекався при температурі 1000°C протягом 4 годин. Щоб змоделювати матеріал для підтвердження його п’єзоелектричних властивостей, було виміряно щільність і досліджено спектри імпедансу на відносну та абсолютну діелектричну проникність; потім ці дані були введені в програму APDL ANSYS. Складність резонансних мод, присутніх у матеріалі обумовлює п’єзоелектричний відгук із кількома піками в широкому діапазоні частот. Ці піки можна використовувати для використання в конкретних ситуаціях, коли необхідна певна частотна характеристика матеріалу.

1. Introduction

Barium titanate ($BaTiO_3$) is a well-known known ceramic that has piezoelectric properties and is therefore used in designs of electromechanical actuators, sensors, and micromotors that need conversion of mechanical energy into electrical energy [1]. Due to its fascinating dielectric and ferroelectric properties, it is used in many energy technologies. Nanoceramics are usually produced by sol-gel, hydrothermal, and solid-state synthesis; solid-state synthesis is preferred due to its cost-effectiveness and ease of operation [2, 3]. The success of any processing technology largely determines the structural, functional as well as the high-end electronic capabilities of the final materials [4]. It is recognized that the synthesis methods also influence the quality of $BaTiO_3$ in its structural, morphological and electrical aspects; there are also methods to analyze these properties, however, in fact, few methods are available to study such properties. X-ray diffraction (XRD) is used to phase analysis of the material, and scanning electron microscopy (SEM) can be employed to observe the changes in the morphology of the material. These are useful for understanding how different synthesis conditions affect the internal structure of materials even at very high pressures [5]. In some cases, additional synthesis methods have been reported for the growth of $BaTiO_3$ under pressure. The dielectric constant of $BaTiO_3$ is most often analyzed using dielectric measurements, which take into account the neutrality of the permittivity [6]. Strain-induced piezoelectricity in $BaTiO_3$ occurs when mechanical deformation changes the polarization and alignment of dipoles, resulting in the generation of an electric charge. This concept is very important for numerous applications such as power devices, motion control, and monitoring systems [7]. The analysis of piezoelectric properties in $BaTiO_3$ has attracted much attention, especially, in connection with the improvement of energy recovery systems and the creation of electromechanical devices [8, 9]. The use of ANSYS APDL to determine the piezoelectric properties of $BaTiO_3$ has also been of interest for many years. In FEA based on ANSYS APDL, mechanical load constants can be added, and the piezoelectric constant is a link and separates the mechanical and electrical properties of $BaTiO_3$ for a better understanding of its electromechanical effect [10].

In this work, barium titanate ($BaTiO_3$) was synthesized and the obtained coatings were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and energy dispersive spectroscopy (EDS) for verification of their structure and composition. A $BaTiO_3$ disc was produced and sintered for impedance spectroscopy measurements and three-point bending assessment. These results were incorporated into ANSYS simulations in order to assess the piezoelectric properties of the material.

2. Experimental

2.1. Preparation of barium titanate nanorods

Hydrothermal processing was utilized to make barium titanate nanoceramics ($BaTiO_3$). Initially, barium chloride ($BaCl_2$, Kishida Chemical), titanium tetrachloride ($TiCl_4$ solution, Sigma-Aldrich), and sodium hydroxide ($NaOH$, Nacalai Tesque, 98%) were used to generate the Ba-Ti-OH precursor. A combination of 1 M $BaCl_2$ (15 ml aqueous solution) and 0.6 M $TiCl_4$ solution (5 ml aq. solution) was created at 25 °C. 40 ml of deionized (DI) water and 10% $NaOH$ were then added to the precursor. The total volume of the original slurry was reduced to 75 milliliters using the hydrothermal technique. To complete the process, the precursor slurry was heated in a 100 ml autoclave lined with Teflon and maintained at 200°C for 24 hr inside the oven. The product was then separated, washed, and dried at 70°C (see Fig.1).

2.2. Characterization of barium titnate nanorods

The crystalline structure and phase of the produced $BaTiO_3$ were verified by analyzing the X-ray diffraction patterns (XRD) (PA-analytical, X-Pert PRO MPD, Cu-K radiation at 30KV). The elemental composition of the produced $BaTiO_3$ nanoparticles was examined using the EDS analysis. To obtain information about the molecular structure, the functional groups and chemical bonds in the $BaTiO_3$ were analyzed using FTIR spectrum spectroscopy. The attenuated total reflectance (ATR) approach was utilized to acquire the FTIR spectra using a Zn-Se crystal in a Nicolet IS50 spectrometer (Thermo Fisher). The spectrometer covered a range of 4500–0 cm^{-1}. Impedance spectroscopy was employed to investigate absolute and relative permittivity. The main goal is to use the obtained impedance data at different frequencies to calculate the relative permittivity of the material (ε'). The sample thickness (d)

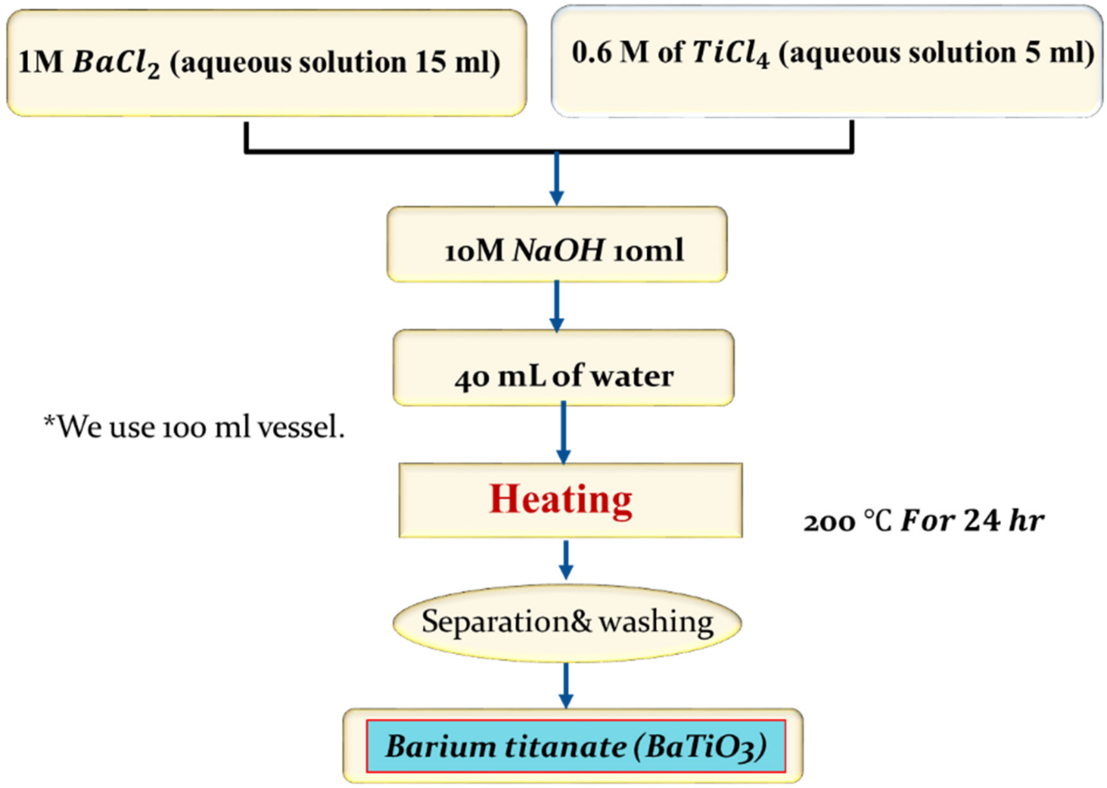

Fig. 1. Illustrative diagram of the stages of $BaTiO_3$ nanorods preparation by using the hydrothermal method

was 1 mm (0.001 m), the disk radius (r) was 0.01 m, and the vacuum permittivity (ε_0) was 8.858×10^{-12} F/m. A press was used to create a barium titanate disc, which was then sintered in a furnace heated to 1000°C. The density was quantified. Barium titanate sample was prepared according to standards (ASTM C1161) for Poisson's ratio and Young's modulus testing.

3. Results and discussion

3.1 Characterization of Barium Titanate

Fourier Transform Infrared (FTIR) spectroscopy was used to detect functional groups within the powder sample (Fig. 2(a)). The resulting FTIR absorbance spectra were recorded in the transmittance mode over the range of 4500–0 cm^{-1}. The functional group of the Ti-O band at 562 cm^{-1} is indicative of the barium titanate structure and is influenced by Ba ions. The functional group of Ba-Ti-O bonds appears in the 1430–1630 cm^{-1} range, while the C-O bands at 1110 cm^{-1} suggest the potential C-C stretching. The C–H band at 2877 cm^{-1} represents the bonding of inorganic groups to titanium. The absence of the Ba-C-O band intensity in the $BaTiO_3$ powder suggests a reduced formation of $BaCO_3$. The OH-OH groups are observable in the 3425 cm^{-1} band. The peroxide synthesis of surface-functionalized barium titanate nanoceramic is revealed by the presence of hydroxyl groups on the (OH) surface functional group [11,12]. Fig. 2(b) presents the X-Ray diffraction (XRD) pattern of the $BaTiO_3$ nanorods (BTNRs). The XRD analysis, consistent with JCPDS no. #892475, reveals the creation of a phase with a lattice parameter of a = 4.0217 Å in the structure of nanorods. The most intense peak (110) is observed at 2θ = 32.17°. Additional peaks detected at 2θ = 22.208° (100), 32.17° (110), 38.898° (111), 45.590° (200), 51.012° (210), 55.927° (211), 65.779° (220), 70.323° (300), and 74.788° (310), further authorize the formation of structure perovskite of barium titanate ($BaTiO_3$) [13,14].

Table 1 shows that oxygen is present in the composition at a weight percentage of 28.30% and an atomic percentage of 67.50%, indicating the formation of oxide in the sample. Titanium is a major component of nanoceramics, supporting the formation of barium titanate and ex-

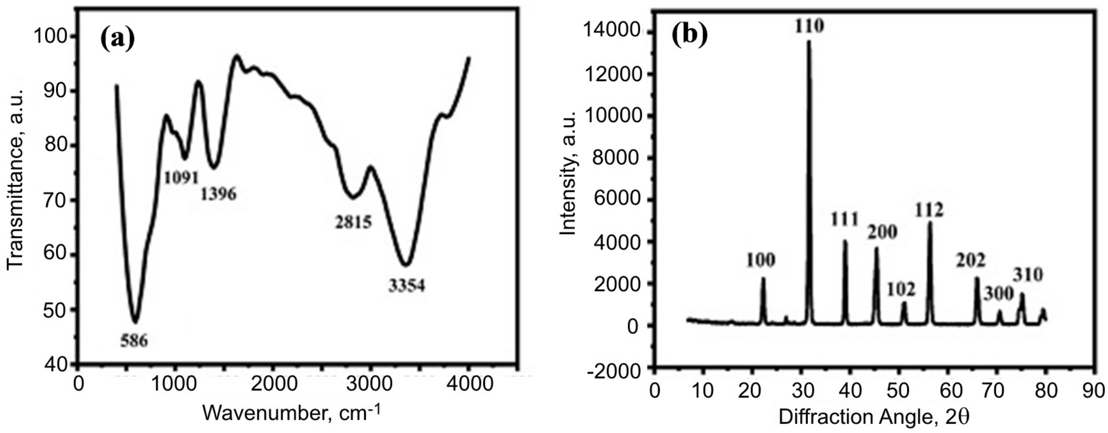

Fig. 2. (a) FTIR spectrum of $BaTiO_3$, **(b)** XRD patterns a tetragonal $BaTiO_3$ nanostructure

hibits weight percentage (24.23%) and atomic percentage (19.31%). The weight percentage of barium is the highest (47.47%), which enhances its prominent role in the synthesis of pure barium titanate.

3.2 Impedance Spectroscopy Analysis of Barium Titanate

The impedance data includes the real part (Z′) and the imaginary part (Z″) at different frequencies (*f*) (see Fig. 6(a)). The real part of the impedance in Ohm·cm^2 is represented by the horizontal axis (Z'), and the imaginary part is represented by the vertical axis (Z"). The results show a gradual decline in the curve, where the imaginary impedance decreases as the real impedance increases. Specifically, the real impedance (Z') increases from 0 to 100,000 Ohm·cm^2, while the imaginary impedance (Z") decreases to negative values reaching –500,000 Ohm·cm^2. This behavior reflects the properties of dielectric materials such as barium titanate nanorods. The observed decrease in imaginary impedance with increasing real impedance may indicate a charging and discharging processes in the dielectric materials, suggesting an interaction between electrons and voids within the material nanostructure. Fig. 6(b) shows the variation of the dielectric constant of barium titanate with frequency. The following relationship, which was obtained from imaginary impedance, was used to compute the dielectric constant [15]:

$$C = \frac{1}{2\pi f\left|Z''\right|}$$

Here C is the capacitance and f is the frequency; the complex impedance is $Z^* = Z' + jZ''$.

Then, we found dielectric constant by the following formula:

$$\varepsilon' = \frac{C.d}{\varepsilon^o.A}$$

Here C is the capacitance; d is the thickness of the dielectric material; A is the area ($A = \pi r^2$); d is the thickness of the sample; and ε^o is the permittivity of free space (8.854 × 10^{-12} F/m). The absolute permittivity (ε) is then calculated as:

$$\varepsilon = \varepsilon_r \times \varepsilon^0$$

It can be seen that the dielectric constant is high at low frequencies and then decreases significantly with increasing frequency until it reaches a quasi-stable value. At higher frequencies, we observe a sharp increase in the dielectric constant, indicating a phenomenon known as resonant frequencies [16,17]. It can be seen that the amplitude is very high at low

Table 1– The content of elements in samples determined by the EDS method (at.%)

Elements	Atomic (%)	Atomic (%) Error	Weight (%)	Weight (%) Error
O	68.0	0.9	28.8	0.4
Ti	19.0	0.2	24.2	0.3
Ba	12.9	0.2	47.0	0.6

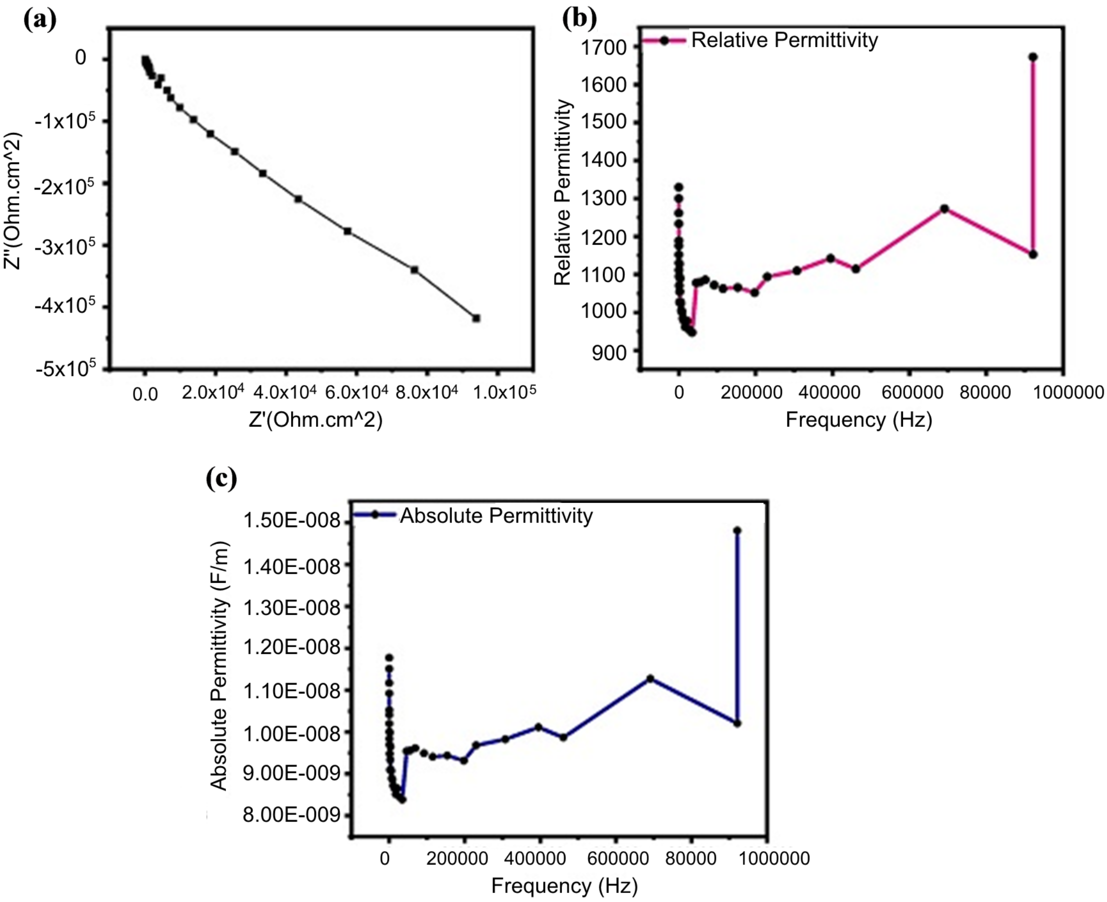

Fig. 3. (a) Impedance spectroscopy of barium titanate powder at different frequencies; (b) relative permittivity *vs* frequency for barium titanate nanopowder; (c) absolute permittivity *vs* frequency for BT

frequencies and then decreases sharply as the frequency increases [18,19].

The results of barium titanate permittivity tests using impedance spectroscopy show a change in relative permittivity at different frequencies. The permittivity initially has a considerable value in low frequency ranges, and diminishes sharply with increasing frequency reaching about 10,000 Hz, which is attributed to the influence of slow polar mechanisms. Then, there are slight variations in the permittivity value in the mid-frequency range – between about 10,000 Hz and 200,000 Hz – where the different polar mechanisms counteract each other. With high frequencies (from 200,000 to 1000,000 Hz) the permittivity shows a huge increase, which means that electronic polarization and resonance effects have taken over [20].

3.3. Three-Point Bending Test

The three-point bending test is a common method for measuring Young's modulus of brittle materials such as ceramics. The sample is placed on two support points, and a load is applied at the midpoint of the sample until it fractures (see Fig. 4). The maximum load and deflection are recorded to calculate Young's modulus. Young's modulus (E) is calculated as:

$$E = \frac{FL^3}{48I\delta}$$

Here E is Young's modulus, F is the force acting on the center of the sample (90 N); L is the distance between the two supports (40mm); I is the reluctance moment of the sample calculated as:

$$I = \frac{bh^3}{12}$$

Here b is the specimen width (horizontal size of the sample 4mm); h is the specimen height 3mm; recorded bending δ=0.148 mm. Based on the results of the three-point bending test, Young's modulus was 90 GPa and Poisson's ratio: 0.3.

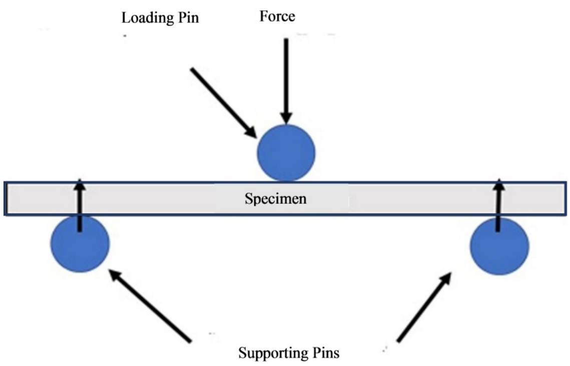

Fig. 4, Three-point bending test for barium titanate

3.4. Modeling by ANSYS APDL for Piezoelectric Testing

Fig. 5 shows the stress distribution in the barium titanate model. Different colors represent different levels of stress; dark blue represents areas of low stress, and lighter colors represent areas of high stress. Maximum stress values are in the dark blue areas. The SXY value means stress in X-Y direction which is negative at the specified point.

The graph in Fig. 6 shows the frequency amplitude (AMPLITUDE) as a function of frequency (FREQ) for an alternating voltage. The frequencies at which the amplitude is greatest are shown. At certain frequencies, clear jumps are observed, indicating the natural frequency characteristics of the model. The largest value of capacitance is about $1.125\times10^{-??}$. The main peaks appear at relatively low frequencies (about 100 Hz and 500 Hz). The voltage reached 768 V at 100 Hz, and the power density reached 5.8, therefore the resistance was 100,000 Ohms. Fig. 7 shows the values of electrical power versus frequency. We conclude that barium titanate withstands varying stresses across the model, and weak or strong points appear clearly at some natural frequencies. Variable peaks indicate the presence of multiple resonant responses. The multiple peaks indicate that barium titanate exhibits a strong resonant response over a wide frequency range. This is common in piezoelectric materials due to the many different modes of vibration in the material. The peaks are likely the result of interactions between electrical and mechanical resonance modes in the material. Every peak indicates a specific natural frequency of the system at which it effectively vibrates. These peaks can include many different vibration modes, such as longitudinal and transverse resonance, as well as surface and bulk modes. Such behavior is beneficial for example in cases where materials or devices need to be designed to operate at their resonant frequency, for instance, in sensors or piezoelectric devices. Barium titanate, for instance, has a complex multi-peaked piezoelectric response over a large frequency range. These peaks can be used for material in cases where a specific frequency response is required. The height of the peaks corresponds to the response level at a given resonant frequency. This suggests a strong response which implies the ability of the material to convert electrical to mechanical energy and vice versa.

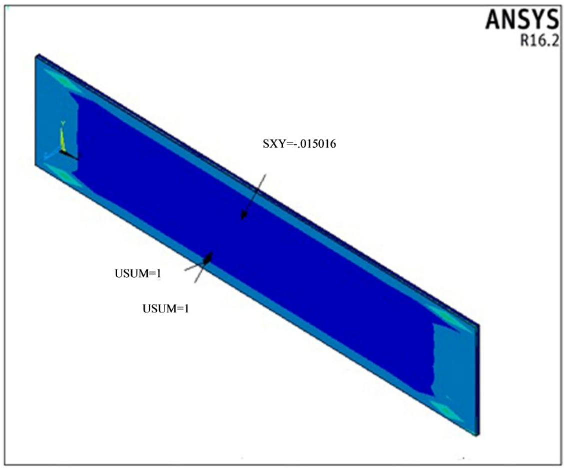

Fig. 5. Stress distribution in the barium titanate model

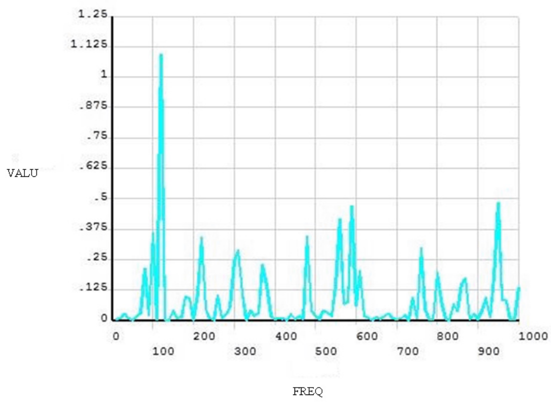

Fig. 6: Amplitude value of voltage depending on frequency

Moreover, barium titanate ($BaTiO_3$) exhibited a multi-peaked piezoelectric effect showing clear resonance peaks centered at frequencies 100 Hz and 500 Hz. This multi-resonance feature is advantageous in applications such as sensors and capacitors that require a certain frequency response. The piezoelectric response of $BaTiO_3$ is complex with several distinct

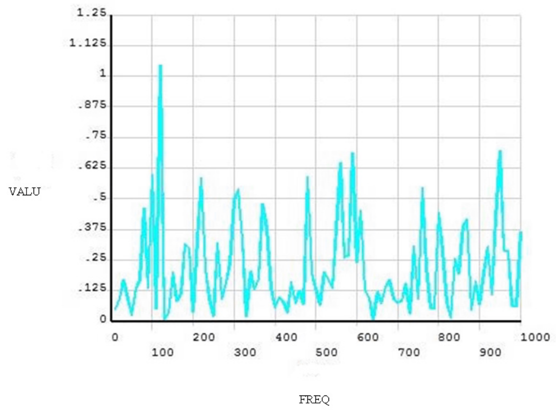

Fig. 7. Amplitude value of power density depending on frequency

peaks occurring where resonance occurs at 100 Hz and 500 Hz reasserting its applicability in areas that require a specific frequency response such as sensors and capacitors [21]. Further, $BaTiO_3$ impedance spectroscopy showed that the relative permittivity gradually decreases with increasing frequency, with stabilization around 10,000 Hz indicating the suitability of $BaTiO_3$ for application as a medium-strength dielectric.

Barium titanate ($BaTiO_3$) has gained recognition for its impressive piezo-activity and features in the manufacture of electromechanical actuators, sensors, capacitors, medical instruments among other applications. Also, the material finds use in energy storage devices and biomedical devices such as sensors which convert mechanical forces to electrical signals due to its excellent dielectric properties and compatibility with living tissues. Nonetheless, $BaTiO_3$ has conventionally some limitations such as requiring high temperature and costly processing techniques.

On the other hand, these limitations have been efficiently eliminated by using the hydrothermal method, since it provides better control over the synthesis conditions. This technique also provides uniformity in the size and shape of $BaTiO_3$ nanoparticle which enhances the uniformity of its piezoelectric properties. However, the lower Curie temperature of $BaTiO_2$ (120°C) limits its use in high-temperature environments compared to lead zirconate titanate (PZT), which has a Curie temperature of around 350°C and exhibits superior stability in high-performance applications [22]. Barium titanate ($BaTiO_3$) is preferred in eco-friendly and medical applications because it is free of lead, unlike PZT (lead zirconate titanate). Given that lead is detrimental to the environment and contributes to health complications, lead-free ceramic materials such as barium titanate $BaTiO_3$ are selected for these applications, especially in practicing medicine or any other applications where humans and the environment have to be considered [23, 24].

4. Conclusion and Future work

In this study, nanostructured $BaTiO_3$ was successfully synthesized using a hydrothermal method and its structural and electrical properties were comprehensively analyzed. The XRD, FTIR, and EDS results confirmed the high purity and crystalline nature of the material. Barium titanate exhibits a multi-peaked piezoelectric response over a wide range of frequencies, reflecting the complexity of its resonant modes. These peaks can be used to exploit the material in applications that require a specific frequency response. $BaTiO_3$ can be used to manufacture highly efficient electrolytic capacitors used in electrical circuits and electronic components. In addition, piezoelectric materials can be useful in developing medical sensors that require converting mechanical signals into electrical signals. This study enhances the understanding of the piezoelectric properties of barium titanate ($BaTiO_3$) and its practical applications, making it very suitable for the field of electromechanical engineering and its multiple applications in industry, robots and sensors.

Further studies should focus on exploring the long-term stability of $BaTiO_3$ in different environmental conditions, such as high humidity and temperature fluctuations. Additionally, the study of the effects of doping $BaTiO_3$ with various elements can further improve its piezoelectric properties. Finally, developing alternative synthesis methods that improve the uniformity and crystallinity of $BaTiO_3$ nanoparticles may lead to better performance in practical applications.

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