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Research Article

Study on Attenuation Coefficients of Cubic BaTiO3

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ABSTRACT

Determining the density, coefficient of thermal expansion of BaTiO3 across range of 400 K to 1075 K is principal goal of the investigation. Coefficient of temperature dependence of density and coefficient of volume thermal expansion of the compound is assessed. Additionally, the research has been broadened to evaluate the linear attenuation coefficient at various γ-energies over a temperature range using value of mass attenuation coefficient.

Keywords: Linear attenuation coefficient, density; thermal expansion; volume thermal expansion coefficient.

1. Introduction

Thermo physical properties, including density (ρ), thermal expansion(α, β), serve to define the characteristics of materials across a range of temperatures. Beyond assessing thermal characteristics, thermal expansion of solids is significant in the selection of materials for various applications. These applications encompass coolant substances, fuel materials pertinent to nuclear reactor safety assessments, and the analysis of heat transfer in molten structural materials following an accident. A comprehensive understanding of temperature variations in many other properties relies significantly on investigating the temperature dependence of above mentioned fundamental characteristics.

Interaction of γ- photons with material over a range of temperature is always a subject of considerable interest and holds significance across multiple scientific fields. To determine the thermophysical properties of the compound γ-radiation attenuation is analyzed at various temperatures using the concept of Drotning[1]. The mass attenuation coefficient (μ_m) for any γ-energy determined in the research makes it easier to analyze the linear attenuation coefficient (μ_l), compound's thermophysical characteristics over a range of temperature. Renu [1] has developed Extended Rigid ion Model and applied for the first time to study the structural, elastic, and thermal properties from 0K to 1000K of $BaTiO_3$ cubic pervoskite material. Thermal expansion studies on ferroelectric materials like $BaTiO_3$ also other materials has been taken up by Radhika [2] over a range of temperature 80K to 800K using dilatometer. Deformation and the thermal expansion coefficient of ceramic samples of (Ba1-xLax) Ti-x/4 O_3 solid solutions (x=0, 0.026 etc) were studied by Gorev, M.V. etal[3] in the temperature range 120-700K using dilatometer. The thermal expansion of the compound has been measured by Megaw [4] between 20°C and 200°C using X-ray powder technique, also Kay and Vousden [5], Rhodes [6] between -160°C and 1200C using single crystal method. The lattice spacing and the linear expansion coefficient has been measured by Bland [7] using X-ray camera over a temperature range 350 °C and 1050°C. Cook et.al [8] studied t he thermal expansion and pyroelectricity of ceramic $BaTiO_3$ was studied. The heat capacity, thermal conductivity and thermal expansion of $BaTiO_3$ based ceramic materials were determined as a function of temperature using Thermo mechanical analysis (TMA) by Yi He [8]. The full-potential linearized augmented plane waves based on DFT using the GGA approximation is applied to study the different properties which includes thermal of different materials by Iles etal [9]. Elmer N. Bunting et al.[10] reported the values of various thermal properties of Ba-St Titanate specimens over different temperature ranges. The coefficient of thermal expansion of Barium Titanate was analyzed by Keyston J.R.G et al [11] over a temperature range -200°C to 100°C. The specific heat and thermal expansion of Barium Titanate ceramics were measured between room temperature and 250°C by Sawada [12] using dilatometer.

Variety of interesting properties of $BaTiO_3$ motivates to use this material in preparing scaffolds for bone tissue engineering - for bone formation, fracture healing, maintaining a charged surface, improving bone cell adhesion and proliferation, bio imaging, anti-cancer drug discovery, also in fabricating non-volatile memory devices, pyroelectric detectors, opto-electronic devices., multilayer ceramic capacitors (MLCCs),transducers and dielectric resonators. This is the reason behind this study.

2. Experimental Details

23.5 gm of $BaTiO_3$ powder is compressed using a hydraulic press. This results in a pellet of 1.342 cm thick. In-depth discussions of the experimental approach and setup specifications have been provided by the authors [15].

To ascertain the (μ_m) values at the energies, the sample is exposed to the γ-radiation from ^{241}Am, ^{137}Cs and ^{60}Co sources. The intensities transmitted are recorded before introducing (I_o) and after introducing (I) the sample during 15 minutes using detection equipment.The temperature dependency of (ρ) and *(α, β)* of specimen has been investigated using (0.66MeV) photons, *(μ_l)* for different energies over a spectrum (400K-1075K), in accordance with the experimental approach given by authors [15]

2.1. Computational Details

Employing Equation (1) of [15], the mass attenuation coefficients (μ_m) for different photon energies are determined. Equations (1–12) of [15] are employed to determine aforementioned thermophysical parameters over a spectrum of temperature. The Coefficient of temperature of density is reported.

3. Results and Discussion

In the current study of $BaTiO_3$ for aforementioned γ--energies, the (μ_m) values are determined using empirical relation (1) of [15] and are presented in Fig.1, also in Table-1 together with the calculated values and values from NIST X-Com. The (μ_m) does not depend on the physical state of the sample; it is also unaffected by temperature. The increase in incoming energy of the photon, reduces the risk of absorption. Taking into account various elements, the estimated uncertainity (*Δ*μ_m) [15], in (μ_m) value in the experimental observations is approximately about 1.19%.

The values of (μ_l) as a function of energy, temperature and (ρ) as a function of temperature have been reported for the first time, no data is available in the literature for comparison. From Table 2, it can be noticed that μ_l decreases with the increase in incident photon energy and temperature. The decrease in μ_l is of about 2.59% over a temperature range for each energy.These variations of μ_l with temperature and at different γ- energies, in the order of increase in energy are obtained from

$$\mu_l(T) = (-1.36 \pm 1.76\times10^{-2})T + (33120 \pm 14.39)$$

$$\mu_l(T) = (-0.0195 \pm 2.52\times10^{-4})T + (476 \pm 0.21)$$

$$\mu_l(T) = (-0.014 \pm 1.8\times10^{-4})T + (336.9 \pm 0.15)$$

$$\mu_l(T) = (-0.013 \pm 1.7\times10^{-4})T + (314.6 \pm 0.14)$$

Barium Titanate (ρ) declines from 6105 kgm^{-3} to 5947 Kgm^{-3} of about 2.59% decrease over a range of Temperature (Table-2 & Fig.2), can be evaluated from

$$\rho(T) = (6222 \pm 2.703) + (-0.2554 \pm 3.3\times10^{-3})T$$

As the mass stays constant while the volume rises with temperature, this leads to a reduction in density.

The density decline is caused by an increase in the equilibrium concentration of thermally generated Schottky defects. Radiation from γ-rays can cause defects. The linear thermal expansion coefficient obtained in this research aligns closely with results from other methods in the literature within the same temperature range (Table-2 &Fig. 3). The *(α)* values obtained in this study are compared with reported values through other method [8]. This indicates that γ-ray radiation has no impact on the density fluctuation. In this research, the (30 mci) source strength and the (~6hrs) irradiation do not seem to have affected the equilibrium concentration of defects in $BaTiO_3$. The coefficient of temperature dependence of density is (-0.2554 Kg $m^{-3}K^{-1}$).

Rise of coefficient of linear thermal expansion (α) can be defined as

$$\alpha(T) = (0.009563 \pm 9.89 \times 10^{-5})T + (4.8 \pm 8.1 \times 10^{-2})$$

Average distance between molecules grows with increase in temperature due to increase in molecular vibrations amplitude, the *(α, β)* values consistently increases. The coefficient of volume thermal expansion increases frob 4.1835x 10^{-5} K^{-1} at 400K to 4.2946x 10^{-5} K^{-1} at 1075K of about 2.66% raise over a temperature range. Rise of coefficient of volume thermal expansion (β) can be defined as

$$\beta(T) = (0.008563 \pm 8.89 \times 10^{-5})T + (4.8 \pm 8.1 \times 10^{-2})$$

Table-1 Comparison of (μ_m) values

μ_m [10^{-3} m^2kg^{-1}]				
Value/γ-Energy (MeV)	Am	Cs	Co	
	0.0595	**0.66**	**1.173**	**1.332**
Expt.	5323	76.5	54.15	50.56
X-Com	5324	76.52	54.16	50.57
Empirical	5325.8	76.5191	54.15724	50.55

Table-2 Thermophysical parameters over a spectrum of temperature

TK	ρ [kgm^{-3}]	μ_l [m^{-1}]				α [$10^{-6}K^{-1}$]		β [$10^{-5}K^{-1}$]
		0.0595MeV	0.66MeV	1.173MeV	1.332MeV	PW	[8]	
393							8.653151	
400	6105	32496.915	467.0325	330.58575	308.6688	9.1		4.1835
450	6095	32443.685	466.2675	330.04425	308.1632	9.3		4.1903
500	6089	32411.75	465.8085	329.7194	307.8598	9.65		4.1944
550	6080	32363.84	465.12	329.232	307.4048	10.1		4.2007
600	6070	32310.61	464.355	328.6905	306.8992	10.5		4.2076
623							10.79844	
650	6057.5	32244.07	463.3987	328.0136	306.2672	11.05		4.2163
673							11.33962	
700	6045	32177.54	462.4425	327.3368	305.6352	11.5		4.225
750	6032	32108.34	461.448	326.6328	304.9779	11.96		4.2341
773							12.29478	
800	6020	32044.46	460.53	325.983	304.3712	12.35		4.2425
850	6005	31964.62	459.3825	325.1707	303.6128	12.84		4.2531
873							13.24668	
900	5991	31890.09	458.3115	324.4127	302.905	13.33		4.2631
950	5978	31820.89	457.317	323.7087	302.2477	13.85		4.2723
973							14.19476	
1000	5965	31751.7	456.3225	323.0048	301.5904	14.45		4.2816

1050	5952	31682.5	455.328	322.3008	300.9331	14.89		4.291
1073							15.1384	
1075	5947	31655.88	454.9455	322.0301	300.6803	15.14		4.2946

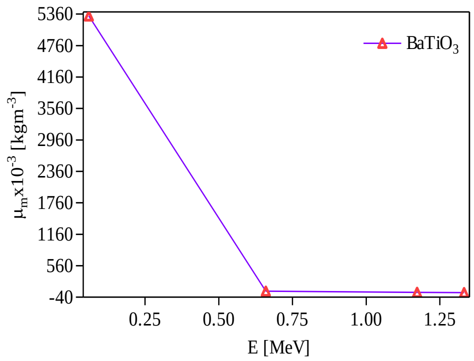

Fig.1 Energy vs Mass attenuation Coefficient

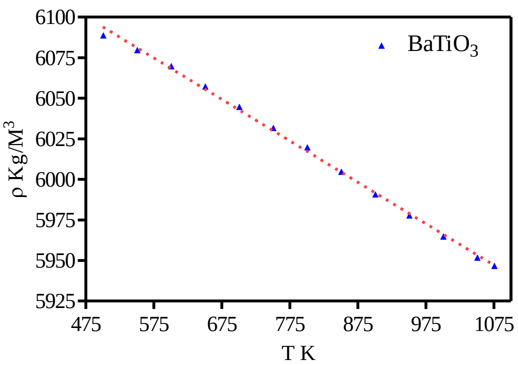

Fig.2. Temperature VS Density (ρ)

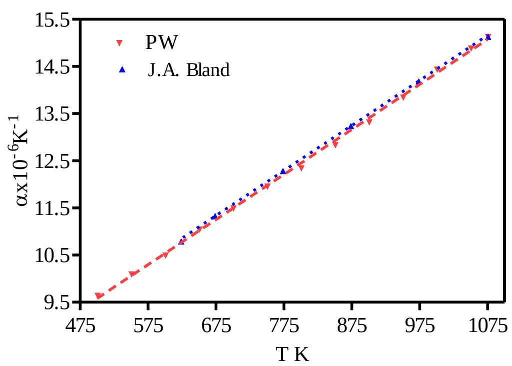

Fig.3. Comparison of temperature VS (α) of [PW] and reported data [8].

4. Conclusions

$BaTiO_3$sample pellet of thickness1.342 cm has been prepared using hydraulic press. A transmitted beam approach is followed in experimental studies on the attenuation of gamma photons at various energies and over a temperature range. The values of (μ_m) at different photon energies were determined. The temperature dependence of values μ_l, ρ, α, β of the sample was presented. It was demonstrated that temperature influence on them through the linear equations. The findings of (α) align well with earlier reported values. γ-ray attenuation method as a function of temperature has been used on $BaTiO_3$ for first time. This marks the initial occurrence of reporting the values of density and linear attenuation coefficient in relation to temperature.

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