



Synthesis and Optical properties of $(\text{Ba}_{(1-x)} \text{Mg}_x \text{Ti}_{(1-x)} \text{Mn}_x \text{O}_3)$ Single Perovskite Oxide

Mohammed Awadh Saeed Al-Ameri¹, Sawsan Ahmed Elhourri Ahmed²
and Musbah Hamed Babikier³

¹Seiyun University- College of Education- Department of Physics, Seiyun – Hadramout - Yemen

²University of Bahri – College of Applied & Industrial Sciences, Department of Physics – Khartoum - Sudan

³AlneelianUniversity- College of Science and Technology, Department of Physics- Khartoum - Sudan

ABSTRACT

Five samples of barium titanate which doped with Mg and Mn ($\text{Ba}_{(1-x)} \text{Mg}_x \text{Ti}_{(1-x)} \text{Mn}_x \text{O}_3$) (where $x = 0.01, 0.2, 0.03, 0.04,$ and 0.05). The samples were synthesized using solid state reaction method, at 1200°C . All samples were investigated by Ultraviolet Visible Spectroscopy. The results of UV technique proved that the absorption and the optical band gap energy of five samples have been increased with increasing of Mg and Mn doping at (3.18, 4.31, 4.35, 4.39, and 4.43 eV). On the other hand, the refractive indexes of the prepared samples have been decreased with dopant (2.31, 2.10, 2.09, 2.089, and 2.083) respectively.

Key words: BaTiO₃, Perovskites materials, UV-visible Spectroscopy, optical Properties

INTRODUCTION

Barium titanate (BT) ceramics were discovered in 1945 by Wainer and Salomon, and they took the researchers attention [1, 2]. These ceramics have attractive properties such as optical, electrical, and structural properties because it is chemically and mechanically very stable, So they can be widely used in many electronic industries like multiplayer capacitors, solar cells, piezoelectric transducers, and gas sensors..etc [3, 4]. These compounds can be prepared in the form of ceramic polycrystalline samples, and they can be exhibited ferroelectric properties at and above room temperature [4]. In general, the Perovskite-structure has a general form ABX_3 and the same crystallographic structure such as BaTiO_3 and CaTiO_3 as shown in figure (1) [5, 6]. In fact, the Perovskite materials can be divided to three types into alkaline metal halide Perovskites, inorganic oxide Perovskites, and organic metal halide Perovskites [7].

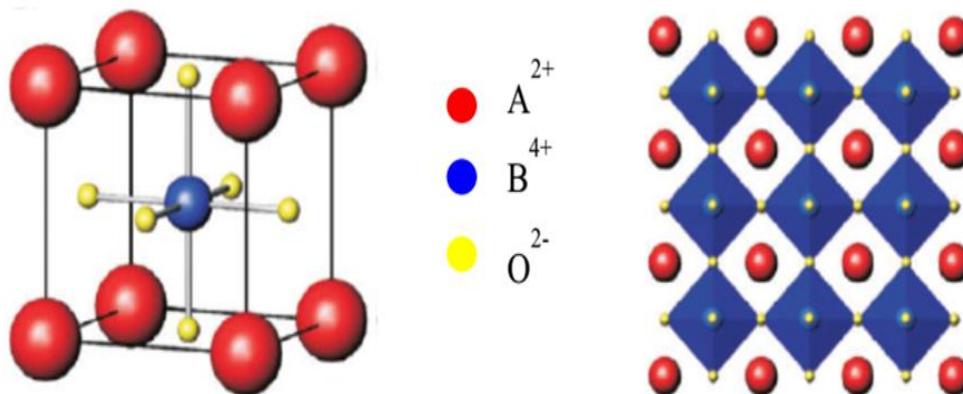


Fig. 1 Ideal cubic Perovskite structure (ABO_3)

The Perovskites compounds have a common structure ABX_3 where ‘‘A’’ and ‘‘B’’ are cations have different sizes and ‘‘X’’ is an anion which bonds to both. The ‘A’ atoms are bigger than the ‘B’ atoms [8]. Also, The A and B locations may be replaced by any metal or semimetal from the periodic table. In all cases, the anion is oxygen, and can be any other could be found at this position [7].

MATERIAL AND METHOD

The Perovskite samples which have a new system $(Ba_{(1-x)}Mg_xTi_{(1-x)}Mn_xO_3)$ (with $x=0.01, 0.02, 0.03, 0.04, 0.05$) were synthesized by solid state reaction method to study the of co-doping magnesium and manganese in two sides of barium titanate ($BaTiO_3$). The starting raw materials were Barium titanate ($BaTiO_3$), Titanium dioxide (TiO_2), Magnesium oxide (MgO), and Manganese dioxide (MnO_2).

All powders were having more than 99% purity. The powders were taken in 2 gm of samples. The powders were thoroughly mixed in a gate mortar with a little amount of acetone for 2hr, after proper mixing, the mixed powders were heated in the laboratory oven at $200^\circ C$ for 4hr. After this heating, the powders were mixed one more time with acetone for 1 hr.

After this step, the powders were culminated at $1200^\circ C$ for 5 hr, and the five solid samples were grinded. The new samples were analyzed using UV-Visible spectroscopy to study some optical properties such as absorption, optical band gap energy, and refractive indexes.

Preparation the New Samples for UV-Visible Analysis

This technique was used with a weight of 0.01 gm and was dissolved in 10 ml of distilled water. The source was calibrated by distilled water. The absorption spectra of the five dissolved samples were recorded in the UV-Visible device.

RESULTS AND DISCUSSION

Absorption

Figure (4) shows the UV-visible spectra of $(Ba_{(1-x)}Mg_xTi_{(1-x)}Mn_xO_3)$ samples as shown at below . The UV-visible analysis provides that the samples absorption increased at different values of maximum wavelengths with dopant of Mg and Mn in $BaTiO_3$ as shown in the table (1) at below:

No.	Sample	Maximum wavelength (nm)	Absorption (a.u)
1	$Ba_{0.99}Mg_{0.01}Ti_{0.99}Mn_{0.01}O_3$	322.6 nm	0.189 (a.u)
2	$Ba_{0.98}Mg_{0.02}Ti_{0.98}Mn_{0.02}O_3$	297.4 nm	0.340 (a.u)
3	$Ba_{0.97}Mg_{0.03}Ti_{0.97}Mn_{0.03}O_3$	293.9 nm	0.346 (a.u)
4	$Ba_{0.96}Mg_{0.04}Ti_{0.96}Mn_{0.04}O_3$	292.4 nm	0.355 (a.u)
5	$Ba_{0.95}Mg_{0.05}Ti_{0.95}Mn_{0.05}O_3$	291.9 nm	0.910 (a.u)

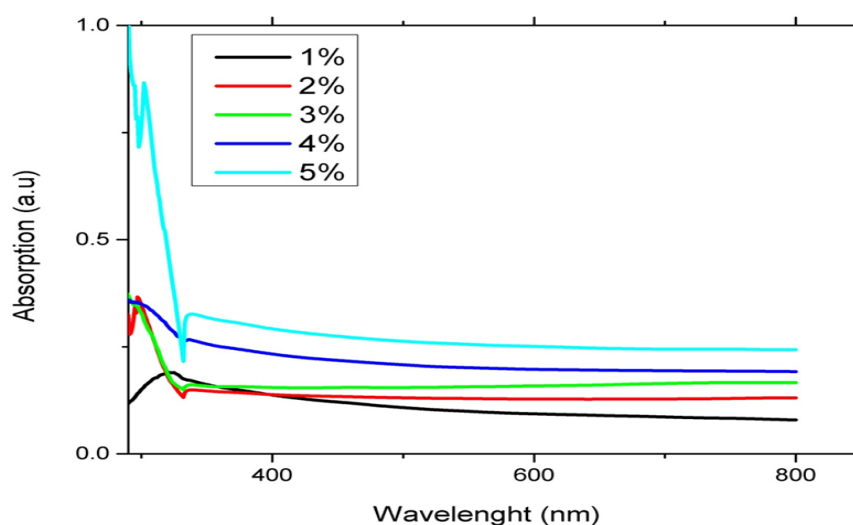


Fig. 4 UV- visible absorption combined for all five samples

Optical Band Gap Energy

The optical band gap energy (E_g) of ($Ba_{(1-x)} Mg_x Ti_{(1-x)} Mn_x O_3$) samples has been calculated by the relation :

$$(\alpha h\nu)^2 = C(h\nu - E_g)$$

Where C is constant, $h\nu$ is a photon energy, and (α) is absorption coefficient. The results confirmed the optical band gap energy increased with contents of Mg and Mn in $BaTiO_3$ as shown in the table (2) at below. The increasing of optical energy band gap may be related to increasing of in grain boundaries and their density duo to heating effect for the crystals of samples.

No.	Sample	Band gab energy (eV)
1	$Ba_{0.99}Mg_{0.01}Ti_{0.99}Mn_{0.01}O_3$	3.18
2	$Ba_{0.98}Mg_{0.02}Ti_{0.98}Mn_{0.02}O_3$	4.31
3	$Ba_{0.97}Mg_{0.03}Ti_{0.97}Mn_{0.03}O_3$	4.35
4	$Ba_{0.96}Mg_{0.04}Ti_{0.96}Mn_{0.04}O_3$	4.39
5	$Ba_{0.95}Mg_{0.05}Ti_{0.95}Mn_{0.05}O_3$	4.43

Refractive indexes

The refractive index (n) was calculated using the relation $n = 3.3668(E_g)^{-0.3224}$

And the refractive indexes decreased with increasing of Mg, Mn concentrations in $BaTiO_3$ as shown in the table (3) below:

No.	Sample	Refractive index
1	$Ba_{0.99}Mg_{0.01}Ti_{0.99}Mn_{0.01}O_3$	2.31
2	$Ba_{0.98}Mg_{0.02}Ti_{0.98}Mn_{0.02}O_3$	2.10
3	$Ba_{0.97}Mg_{0.03}Ti_{0.97}Mn_{0.03}O_3$	2.09
4	$Ba_{0.96}Mg_{0.04}Ti_{0.96}Mn_{0.04}O_3$	2.089
5	$Ba_{0.95}Mg_{0.05}Ti_{0.95}Mn_{0.05}O_3$	2.083

The refractive index of pure barium titanate is 2.360, and the decreasing of reflective index of dopant in all samples above may be related to the samples became more transparent with increasing of Mg and Mn contents.

CONCLUSION

Five samples of single Perovskite oxides of Mn ($Ba_{(1-x)} Mg_x Ti_{(1-x)} Mn_x O_3$) where $x=0.01, 0.2, 0.03, 0.4,$ and $0, 05$ have been successfully prepared using solid state reaction method, and their optical properties were studied by UV-Visible spectroscopy technique. The results of UV-visible spectra for indicate that the samples have a high absorbance in (0.189, 0.340, 0.346, 0.355, and .0910 a.u), and the optical band gap energy increased with dopant of Mg and Mn (3.18, 4.31, 4.35, 4.39, and 4.43 eV) respectively. Also, the reflective index of all samples deceased with doping of Mg and Mn (2.31, 2.10, 2.09, 2.089, and 2.083) respectively. The prepared material closed to insulator material because the results of optical band gap increased with dopant of Mg and Mn at $BaTiO_3$.

REFERENCES

- [1]. Popovici, D., M. Okuyama, and J. Akedo, Barium Titanate-Based Materials—a Window of Application Opportunities. *Ferroelectrics-Material Aspects*, by Mickaël Lallart, IntechOpen, London, 2011: p. 279-304.
- [2]. Lee, T. and I.A. Aksay, Hierarchical structure–ferroelectricity relationships of barium titanate particles. *Crystal Growth & Design*, 2001. 1(5): p. 401-419.
- [3]. Ayub, N., et al. Characteristics of Porous Sb-Doped Barium Titanate Ceramics Fabricated by Adding Graphite. in *Advanced Materials Research*. 2015. Trans Tech Publ.
- [4]. Vijatović, M., J. Bobić, and B. Stojanović, History and Challenges of Barium Titanate: Part I. *Science of Sintering*, 2008. 40(2).
- [5]. Bradley, K., *Crystal structure prediction for complex modular materials*. 2017, University of Liverpool.
- [6]. Jeon, N.J., et al., Compositional engineering of perovskite materials for high-performance solar cells. *Nature*, 2015. 517(7535): p. 476.
- [7]. Chen, Y., et al., Large-area perovskite solar cells—a review of recent progress and issues. *RSC advances*, 2018. 8(19): p. 10489-10508.