

# Effect of KOH Concentration on the Optical and Structural Properties of Perovskite CaZnO<sub>3</sub> Thin films

<sup>1</sup>Raed H. AL-saqa, <sup>2</sup>I. K. Jassim

<sup>1,2</sup>Department of Physics, College of Education for Pure Science, Tikrit University.iq <sup>1</sup>Email: raed.h.alsaqa@st.tu.edu.iq <sup>2</sup>E-mail: ismail\_khalil1956@yahoo.com

## ABSTRACT

#### Article Info

Publication Issue Volume 10, Issue 1 January-February-2023 Page Number 33-37 Article History Accepted: 01 Jan 2023 Published: 06 Jan 2023 A scanning electron microscope, X-ray spectrum, and UV spectrometer have been used in the examination of CaZnO<sub>3</sub> perovskite thin films. Chemical Spry Pyrolysis (CSPD) technique was used in the preparation of the films from a mixture including different concentrations of KOH and a constant substrate temperature. The effect of KOH concentration was clear on the film's transmittance, absorbance, and energy gap. The energy gap varied from 2.75 eV with 0.6 gm of KOH, up to 2.95 eV for 1.2 concentration, and finally, the energy gap became 3.1eV with 1.8 gm of KOH. In addition, the average grain size also decreased with KOH concentration, from 116 nm to 92 nm. **Keywords:** CaZnO<sub>3</sub>. Perovskite, energy gap, grain size, UV- spectrophotometer

## I. INTRODUCTION

Perovskite materials regarded are as reliable substitutes for silicon and germanium in semiconductors. Although perovskite has a variety of configurations, the most prevalent one is ABX<sub>3</sub>, which has five atoms [1]. where diameter of "A" element is rather large. "X" is an oxygen atom, which can either be a halogen or a nitrogen atom [2], and "B" is a cation of small dimension from a "transitional or noble metal" [3].



Figure. 1 perovskite's perfect stricture, "ABX<sub>3</sub>," which creates a three-sided network, "BX6"[4].







Figure.2 CaTiO<sub>3</sub> pervoskite structure a: The perfect perovskite structure is ABX<sub>3</sub>, b: The octet of existence deviates to varying degrees resulting in reduced symmetry compared to the original cube.[5]

Various techniques, including chemical bath deposition (CBD) [6], chemical vapor deposition (CVD) [7], the silar method [8], spin coating method [9], and spray pyrolysis deposition (SPD) [10], can be used to make pervoskite quickly. Perovskite materials have been utilized in a variety of industrial applications, such as transistors, memory, and capacitors [11, 12], light emitting diodes (LEDs) [13], radiotherapy dose measurement [14], transparent ceramics [15], photovoltaic cells [16], fuel cells [17], and in the preparation of superconducting materials at relatively high temperatures [18]. The structural characteristics of these layers were examined using a scanning electron microscope (SEM) and X-ray spectrum, the transmittance, absorbance, refractive index, and extinction coefficient have also been investigated using UV-spectrophotometer. A different concentration of precursor KOH was used to prepare thin films of inorganic perovskite structure CaZnO3 which has lattice parameter "a = 5.953937, b = 5.807390, c =7.171034,  $\alpha = \beta = \gamma = 90^{\circ}$ [19].

#### II. METHODS AND MATERIAL

Glass slides were used as the substrate for the films' deposition. They were cleaned using ultrasound, methanol, distilled water, and numerous other cleaning agents before being allowed to dry. CaZnO<sub>3</sub> thin films have been prepared using constant concentrations of calcium chloride (CaCl<sub>2</sub>) and zinc chloride (ZnCl<sub>2</sub>) with different concentrations of potassium hydroxide (KOH), as shown in table 1.

Tab.1 Concentration of CaCl<sub>2</sub>, ZnCl<sub>2</sub> and KOH

	CaCl <sub>2</sub> gm	ZnCl <sub>2</sub> gm	KOH gm
1 <sup>st</sup> Concentration	0.6	0.6	0.6
2 <sup>nd</sup> Concentration	0.6	0.6	1.2
3 <sup>rd</sup> Concentration	0.6	0.6	1.8

Solutions of CaCl<sup>2</sup> and ZnCl<sup>2</sup> compounds were added concurrently to different concentrations of KOH solution after each component was dissolved in 50 ml of distilled water. For one hour at 80 °C, the mixture was agitated with a magnetic stirrer. Using chemical Spry pyrolysis deposition, the latter solution was utilized to create thin films of CaZnO<sub>3</sub> on the glass slides at 150 °C. The substrate temperature during the



deposition process was maintained at 150 °C, with an atmospheric pressure of 7.5 bars and 10 spray steps lasting 5 seconds.







**Figure.3** effect of concentration on the optical properties a. energy gap b. absorption c. transition

Images of the layers taken using a scanning electron microscope reveal that the grains' sizes are related to the concentrations of their predecessors. As the grains aggregate and grow, the first concentration image depicts the formation of a nanoroad structure with a diameter of approximately 90-125 nm, the second concentration image depicts the formation of cubic-shaped grains, and the third concentration image depicts the formation of uniformly distributed grains with a size of approximately 80 nm.

The presence of multiple peaks belonging to the single crystal phase with different intensities at the same angle  $(2\theta)$  in addition to the appearance of additional peaks due to the different orientation in the structure of the prepared films' structures are all signs that the films are all amorphous, according to the x-ray spectrum figure (4).



Fig.4 Scanning Electron Microscope images and X-ray spectrums of the layers prepared from different concentrations of KOH (a-1<sup>st</sup> concentration; b- 2<sup>nd</sup> concentration; c- 3<sup>rd</sup> concentration)

No. concentration	Average grain size nm	energy gap eV
1¤ Concentration	116.7	2.7
2 <sup>nd</sup> Concentration	111.5	2.95
3rd		

**Table (2)** show the variation of grain size andenergy gap with KOH concentration

#### **III. RESULTS AND DISCUSSION**

Concentration

92.4

3.1

To create thin films of the CaZnO<sub>3</sub> structure, a combination of various concentrations of KOH with constant constration of CaCl<sub>2</sub> and ZnCl<sub>2</sub> were used. Using a spectrophotometer, a scanning electron microscope (SEM), and an X-Ray spectrum, the layers' optical and structural characteristics were assessed.

For all concentrations, the optical characteristics clearly vary, with the transmittance decreasing as the KOH concentration increases while the absorbance increasing, proportional to concentration spatially from wave length 300 nm to 550 nm as shown in figure(3).The energy gap was 2.7 eV for the first concentration (lowest concentration), increased to 2.95 eV for the second concentration, and eventually became 3.1 eV for the third concentration figure (3-a), which is close to the ZnO optical band [20], one of the components of CaZnO3. This mean the band gap increase with increasing concentration of (KOH). The structure and grain size of prepared films are continuously changing, which causes a variation in the energy gap, figure(3-a).

### IV. CONCLUSION

Transmittance and absorbance vary according to the variation concentrations of KOH with fix

concentrations of CaCl2 and ZnCL2. The absorbance and transmittance index spectrum exhibits steady values for all concentrations along the range (300–550 nm) before decreasing over the range (550-600 nm). The band gap was 2.7 eV for the initial concentration, 2.95 eV for the second concentration, and finally 3.1 eV for the third concentration. The structure of the films varies greatly throughout concentrations, as seen in scanning electron microscope images. X-ray spectrum show that the layers are completely crystalline, and peaks for all concentrations appear at the same  $2\theta$  with different intensities. In addition, the calculated grain size decreased with KOH concentration increasing.

Finally, the outcomes demonstrated the potential for producing a thin film from the semiconductor Pervoskite CaZnO<sub>3</sub>, which makes it suitable for application in the production of solar cells and diodes.

#### V. Acknowledgements

In particular, we appreciate the assistance with the XRD and SEM tests provided by Dr. Mohammad M. Unise from the University of Mosul, Dr. Sattar J. Kasim, and Mazin A. Mahdi from the University of Basra.

#### **VI. REFERENCES**

- K. Frohna, Samuel D. Stranks, (2019).in Handbook of Organic Materials for Electronic and Photonic Devices (Second Edition),
- [2]. D. Chenine.(2019). Ab-initio study of structural, optoelectronic, thermodynamic and magnetic properties of Perovskite, doctoral thesis, Abdelhamid Ibnbadis University. Mostaganem,
- [3]. K. Jemli. (2016). Synthesis and self-assembly of perovskite molecules for photonics and labeling, doctoral thesis, University Paris-Saclay. Paris.
- [4]. Kumar Shaw B, Castillo-Blas C, Thorne M, Gómez MLR, Forrest T, Lopez MD, et. al.

(2021);Principles of Melting in Hybrid Organic-Inorganic Perovskite and Polymorphic ABX3 Structures. ChemRxiv. Cambridge: Cambridge Open Engage.

- [5]. Brooks K. Perovskite [Internet]. Wiley online library. (2020) [cited 15 December 2020]. Available from: https://onlinelibrary.wiley.com/doi/abs/10.1111 /gto.12299
- [6]. Iman Ahmed Younus, Anwar M. Ezzat & Mohammad M. Uonis.(2020). Preparation of ZnTe thin films using chemical bath deposition technique. Nano composites, 6:4, 165-172, https://doi.org/10.1080/20550324.2020.1865712
- [7]. Sun, L., Yuan, G., Gao, L. et al. Chemical vapour deposition. Nat Rev Methods Primers 1, 5 (2021). https://doi.org/10.1038/s43586-020-00005-y
- [8]. Alaa.A.F., Husain Suhayla, Win Zuha Wan Hasan, "Transparent solar cell using spincoating and screen printing", Pertanika journal of science and technology, Vol 25, pp 225-234.2017.
- [9]. Takeo Oku, Junya Nomura, Atsushi Suzuki, Hiroki Tanaka, Sakiko Fukunishi, Satoshi Minami and Shinichiro Tsukada. (2018). "Fabrication and Characterization of CH3NH3PbI3 Perovskite Solar Cells Added with Polysilanes", International Journal of Photo energy, vol. 2018, Article ID 8654963, 7 pages, https://doi.org/10.1155/2018/8654963
- [10].Perednis, D., Gauckler, L.J. (2005). Thin FilmDepositionUsingSprayPyrolysis.JElectroceram14,https://doi.org/10.1007/s10832-005-0870-x.
- [11]. H. Bali, and B. Raveau. (1983). Mat. Chem. and Phys., 8469.
- [12]. G. Xing, N. Mathews, S. Sun, S. S. Lim, Y. M. Lam, M. Grätzel, et al. (2013)."Long-range balanced electron-and hole-transport lengths in organic-inorganic CH3NH3PbI3," Science, vol. 342, pp. 344-347.

- [13]. X. Che, Étude. (2018). theory of halogenated perovskite materials, doctoral thesis, University of Rennes 1. Rennes.
- [14]. Tsai H, Liu F, Shrestha S, Fernando K, Tretiak S, Scott B, et al. (2020). A sensitive and robust thin-film x-ray detector using 2D layered perovskite diodes. Sci Adv 6(15):815. doi:10.1126/sciadv.aay0815.
- [15]. Ph. Courty, H. Ajot, Ch. Marcilly, and B. Delmon. (1973). Powder Technology,7, 21.
- [16]. A. Kunioka and Y. Sakai. (1965). Solid-State Electronics, 8, 961.
- [17]. N. Q. Minh. (1993). Ceramic fuel cells, J. Am. Ceram. Soc. 76, 563.
- [18]. S. Gariglio and J.M. Triscone. (2011). Compte Rendu Physique, 59.
- [19]. https://oqmd.org/materials/structure/2006046. 1/11/2022.
- [20]. Bakha, Yamna & Khales, Hamza & Smatti, A & SERHANE, Rafik. (2020). Structural and Optical Properties of Nanoparticle ZnO Deposited by Spray Pyrolysis, Algerian Journal of Research and Technology, ISSN : 2543-3954, A.J.R.T Volume 4 (N° 1), (2020) 1-7. Centre for Development of Advanced Technologies, Cité 20 Août 1956, Baba Hassen, BP. 17, Algiers DZ-16303, Algeria.

# Cite this article as :

Raed H. AL-saqa, I. K. Jassim, "Effect of KOH Concentration on the Optical and Structural Properties of Perovskite CaZnO3 Thin films", International Journal of Scientific Research in Science and Technology (IJSRST), Online ISSN : 2395-602X, Print ISSN : 2395-6011, Volume 10 Issue 1, pp. 33-37, January-February 2023. Available at doi : https://doi.org/10.32628/IJSRST229692 Journal URL : https://ijsrst.com/IJSRST229692