

Preparation and Characterization of ZrO₂ -PVA Doped TiO₂ Nanocomposite in Solar Cell Application

M.N. Jothi¹, IG.Jeya Jothi², V.Hemalatha³, R.Rajammal⁴

^{1,2}Assistant Professor, Department of Physics, Sakthi college of arts and science for women, Dindigul, India

³II M.Sc physics, Department of physics, Sakthi college of arts and science for women, Dindigul, India

⁴M.V. Muthaiah Government Arts College, Dindigul

ABSTRACT:

The objective of the project is to presents the research results of PVA-Zr-Ti nanocomposite synthesis. Polymer nanotechnology is a growing technology which is really useful in solar cells. Solar cells which are made from using nanocomposite were environmentally friendly and uses natural methods to prepare nanocomposites. Among the all zirconium and titanium nanoparticles draws more attention due to their significant bio compatible, electrical, mechanical and optical properties. Polyvinyl alcohol is a semicrystalline and water-soluble polymer with a non-toxic nature, biocompatible and has better chemical resistance. The PVA-Zr-Ti nanocomposite prepared using solution casting method. Which is an effective and rapid method to prepare nanocomposite. The prepared sample characterized by FTIR, XRD and EDX. The FTIR analysis displays the functional groups of nanoparticles and the structural properties were given by XRD.To determine the types of the elements, present in the compounds, the EDX analysis of all the samples was carried out.

Index Terms: Polyvinyl alcohol, Zirconium, Titanium, Nano composite, Nano particles, Solar cells, Solution casting method, FTIR, XRD, EDAX.

INTRODUCTION

Nanotechnology generates interest among the researchers in recent years due to their distinguished properties and various applications in fields of industrial, medical, commercial and also in solar technology. Development of applications incorporating Semiconductor nanoparticles to be used in the next generation of products, such as solar cells, display technology, lighting, biological imaging such as quantum dots. Nanoparticles are tiny particles; the size of nanoparticles ranges from 1 to 100 nm. They can be classified into different classes based on their properties, size and shape. The nanoparticles possess unique and different properties due to their nanoscale size. Their optical properties are reported to be dependent on the size, which imports different colours due to absorption in visible region. Their reactivity, toughness and other properties are also depending on their unique size, shape and structure. Due to these unique characteristics the nanoparticles are widely used in commercial and domestic applications.

Polyvinyl alcohol (PVA) also referred to as PVAL, PVOH, or POVAL is a highly biocompatible, synthetic-nontoxic, and highly water-soluble polymer. It can be used as the host of material for composite corresponding to good thermal stability and resistance. Also, polyvinyl alcohol nanocomposites are easy to produce. Zirconium comes under the type of strong transition metals. They have the specific properties such as toughness, high tensile strength, and hardness. Due to these properties zirconium nanoparticles are widely used. Also, zirconium naturally available in nature abundantly. The various properties and characteristics of zirconium allows it to be used in wide range of application such as ceramic making, porcelain, in making abrasive, insulating and fire-retarding materials. Bio synthesized Zr and Ti nanoparticles along with PVA can give a nanocomposite which has significant applications in solar cells. This study was undertaken with the objective to produce PVA – Zr doped with Ti nanocomposite in a more natural and eco-friendly method.

EXPERIMENTAL TECHNIQUES

1. Synthesis of zirconium nanoparticles:

Zirconium nanoparticles are synthesized using green synthesis nano technology. About 50g of *Andrographis paniculata* taken into a beaker with 200 ml of deionized water, then it was heated in a hot plate for 40 minutes at 60 deg temperature. Then the leaf extract was filtered and about 50 ml of leaf extract taken into a beaker. And 5 M of zirconium salt added to 200 ml deionized water, this solution stirred for an hour until the zirconium particles become solution. The measured 50 ml of *Andrographis paniculata* added to the zirconium solution. The colour of final solution is white. After 30 minutes the solution taken out from stirrer, and leaving the particles to settled down for 12 hours. Then the solution was placed in an oven to prepare nanoparticles.

2. Synthesis of Titanium nanoparticles:

Titanium nanoparticles prepared in a similar way as Zirconium nanoparticles. About 50g of *Solanum trilobatum* taken into a beaker with 200 ml of deionized water, then it was heated in a hot plate for 40 minutes at 50 deg temperature. Then the leaf extract was filtered and about 50 ml of leaf extract taken into a beaker. And 5 M of titanium salt added to 200 ml deionized water, this solution stirred for an hour until the titanium particles become solution. The measured 50 ml of *Solanum trilobatum* leaf extract added to the titanium solution. The colour of final solution is white. After 30 minutes the solution taken out from stirrer, and leaving the particles to settled down for 12 hours. Then the solution was placed in an oven to prepare nanoparticles.

3. Preparation of Polymer:

The Polymer was prepared from polyvinyl alcohol. About 0.7 g of polyvinyl alcohol measured and taken into a beaker, now the measured PVA added to 10 ml of deionized water. The salt solution stirred for 5 hours. In the polyvinyl alcohol solution 0.3 g of prepared zirconium nanoparticles added, it takes an hour to blend the zirconium nanoparticle with polyvinyl alcohol. After one hour 0.5 g of prepared titanium nanoparticles added to the PVA-Zr solution and the solution stirred for another hour. Finally, the solution casted in a glass petri dish and kept in a clean place at room temperature for 48 hours. To remove the impurities the petri dish washed with deionized water and cleaned by applying ethanol on the surface. Finally, the polymer film carefully removed from petri dish. The colour of final solution is white. The polymer film was formed by solution casting method. The characterization of synthesized

Polymer was done by UV-spectroscopy, Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD). To determine the types of the elements, present in the compounds, the EDX analysis of the samples was carried out.

RESULT AND DISCUSSION

FTIR

The functional groups of nanocomposites consisting the elements of PVA, Zirconium and Titanium were studied using Fourier Transform Infrared Spectroscopy. FTIR analysis over the region of $400\text{-}4000\text{cm}^{-1}$ wavelength were presented. Polyvinyl Alcohol has distinct bands at $2800\text{-}3000\text{cm}^{-1}$, $3200\text{-}3570\text{cm}^{-1}$ and $1000\text{-}1200\text{cm}^{-1}$ which corresponds to **Alkyl stretching groups, hydroxyl groups, hydrogen bonded groups and C-O Stretching bonds** respectively. The spectra of nanocomposite film having range 444cm^{-1} is the metal-oxygen group (**Zr-O**). The peak at 3243cm^{-1} of pure PVA film is shifted to higher wave number 3273cm^{-1} and it is due to the presence of **ZrO₂ into polymer matrix**. hence these peaks confirm the presence of Zirconium nanoparticles. The **TiO₂** stretching is found at the peak value of 756cm^{-1} which confirms the presence of Titanium nanoparticles in nanocomposite.

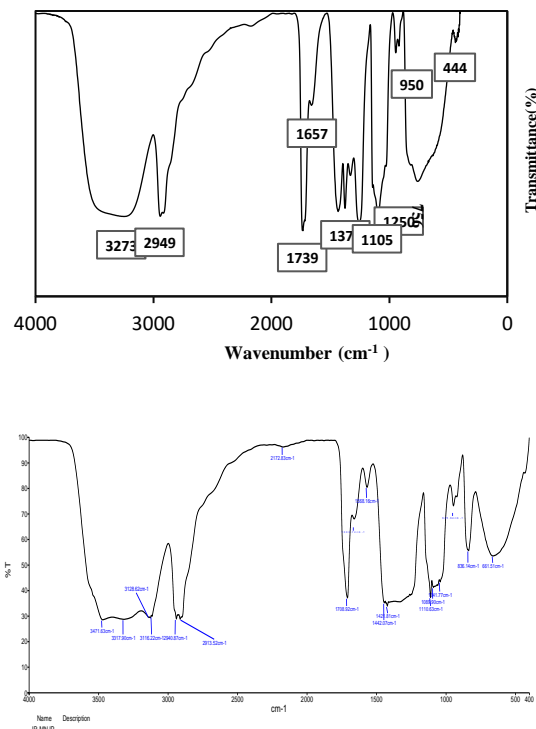


Fig (b) FTIR Spectra of Pure PVA.

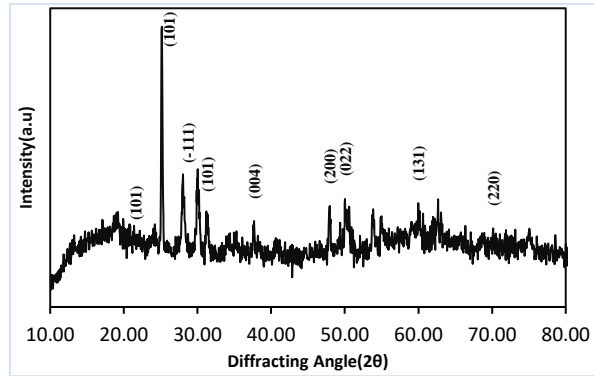
Fig (a) FTIR Spectra of Pva-ZrO₂ doped with TiO₂ nanocomposite film

XRD(X-RAY DIFFRACTION)

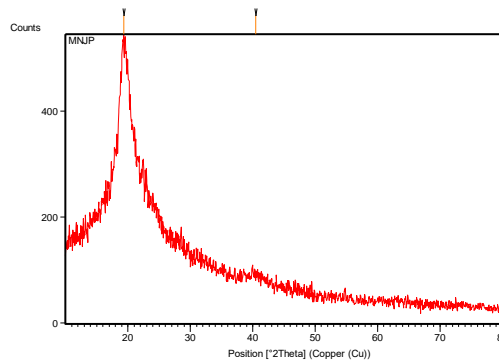
XRD analysis was performed to study the crystalline structure. The Debye Scherrer equation, $D = K\lambda / \beta \cos\theta$, is used to calculate the crystalline size of the nanoparticles, where D is the nanoparticles crystalline size, K represents the Scherrer constant (0.98), λ denotes the wavelength (1.54), β denotes the full width at half maximum (FWHM).

The diffraction peak appears at around $2\theta = 19.01^\circ$ (101), which confirms the presence of PVA. Some of the peaks of Zr at $28.01^\circ, 31.28^\circ, 50.20^\circ, 59.69^\circ$ & 75.01° corresponding to the hkl values (-

111),(111),(002),(131) and (220) respectively. This confirms the zirconium nanoparticles in the film. These peaks are belonging to monoclinic structure. The peaks at 25.14°, 37.63°, 53.82°, 55.04° and 62.52° corresponding to the hkl values (109),(004),(105),(211) and(116) which confirms presence of titanium nanoparticles in pva-zr-ti nanocomposite. These peaks are corresponded to tetragonal anatase phase structure.



Fig(a).XRD Pattern of PVA-Zirconium doped Titanium nanocomposite



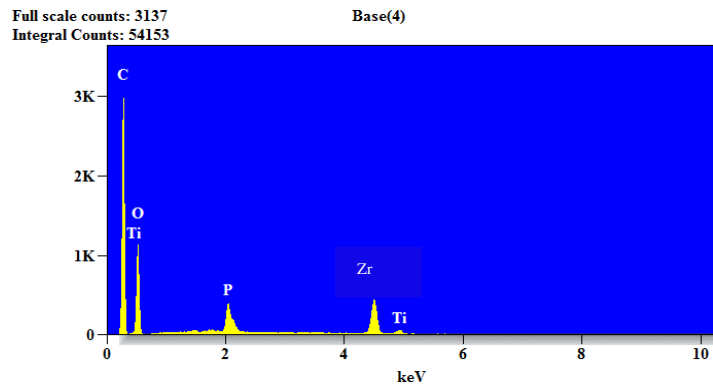
Fig(b) XRD pattern of pure PVA

The XRD pattern of pure PVA polymer indicates a broad peak at position of 19.33° which is corresponding to non-crystalline or amorphous behaviour of polymer .

Pos. [°2Th.]	Height [cts]	FWHM Left [°2Th.]	d-spacing [Å]	Rel. Int. [%]
19.3315	287.63	1.3776	4.59164	100.00
40.5145	13.81	3.1488	2.22663	4.80

EDX(ENERGY-DISPERSIVE X-RAY SPECTROSCOPY)

EDX analysis of the samples was carried out to determine the types of the elements present in the compounds, the following graph confirms the elements present in the composite. EDX spectra of nanocomposites obtained from Pva-ZrO₂ doped with TiO₂ nanoparticles are shown and in Fig. As seen from the EDX results, the peaks in the spectrum confirm the formation of from Pva-ZrO₂ doped with TiO₂ nanocomposites in the presence of PVA and Zr. Carbon and oxygen peaks are due to polymer matrix substrate. which confirms the presence of Nanoparticles



Quantitative Results

Element	Net Counts	Weight %	Atom %	Atom % Error	Formula
C	17594	40.28	50.68	± 0.38	C
O	6967	47.80	45.15	± 0.57	O
P	3083	2.41	1.18	± 0.04	P
Ti	5803	9.51	3.00	± 0.04	Ti
Zr	5975	9.76	4.00	±0.03	Zr
Total		100.00	100.00		

The quantitative results of EDX analysis described in the above table. it provides the details of elements present in the Nanocomposite.

CONCLUSION

The Pva-ZrO₂ doped with TiO₂ nanocomposite film were produced using the solution method, As the polymer had a wide range of application especially on the field of solar cell technology it is significant to study about polymer nanocomposites and produce polymer nanocomposites in a natural and efficient way. The above method provides a solution to produce nanocomposite in a simple and rapid way. The characteristics of Pva-ZrO₂ doped with TiO₂ nanocomposite were studied using FTIR , EDAX and XRD.FTIR studies shows the interaction between the -OH group of PVA with the Zr-O and Ti-O through hydrogen bonding. XRD analysis gives the detailed information about the crystalline structure of PVA, Zirconium and Titanium compounds. The EDX analysis gives data of the presence of PVA, Zirconium and Titanium compounds. These results suggest the Ti and Zr can be used as effective nanofiller for Polymer composite.

REFERENCES

1. Tayser Sumer Gaaz ,Abu Bakar Sulong, Majid Niaz Akhtar, Abdul Amir H. Kadhum, Abu Bakar Mohamad, Ahmed A. Al-Amiery. (2015). Properties and Applications of Polyvinyl Alcohol, Halloysite Nanotubes and Their Nanocomposites, journal of MDPI, 20(12), 22833-22847.
2. M.H. Dwech, M.A. Habeeb, A.H. Mohammad. (2023). Fabrication and Evaluation of optical characteristics of (PVA-MnO₂-ZrO₂) nanocomposites for Nanodevice in Optics and Photonics, Journal of Physics, DOI:10.1547/ujpe67.10.757.

3. Couto de Azevedo Gonçalves Mota, R. , Oliveira da Silva, E. and Rodrigues de Menezes, L. (2018) Effect of the Addition of Metal Oxide Nanoparticles on the Physical, Chemical and Thermal Properties of PVA Based Nanocomposites. *Journal of scientific research*, 9, 473-488.
4. Manjunath, A. , Irfan, M. , Anushree, K. , Vinutha, K. and Yamunarani, N. (2016) Synthesis and Characterization of CuO Nanoparticles and CuO Doped PVA Nanocomposites. *Journal of scientific research*, 6, 263-273.
5. Ye, M., Mohanty, P. and Ghosh, G. (2014) Morphology and Properties of Poly Vinyl Alcohol (PVA) Scaffolds: Impact of Process Variables. *Materials Science and Engineering: C*, 42, 289-294.
6. Mohanapriya, S., Mumjitha, M., Purnasai, K. and Raj, V. (2016) Fabrication and Characterization of Poly (vinyl alcohol)-TiO₂ Nanocomposite Films for Orthopedic Applications. *Journal of the Mechanical Behavior of Biomedical Materials*, 63, 141-156.
7. S.Ashok, Raymond T.Fonash, Stephen Joseph Fonash, (2023),solar cell electronics, Britannica, <https://www.britannica.com/technology/solar-cell>.
8. Nancy Haegel, Photovoltaic Applications , NREL nrel.gov <https://www.nrel.gov>.
9. Polymer Description,Examples,Types, Material, Uses, & Facts Encyclopedia Britannica, <https://www.britannica.com>.
10. Pedro Henrique CuryCamargoKestur, Gundappa Satyanarayana, Fernando Wypych, (2016), Nanocomposites: synthesis, structure, properties and new application opportunities, <https://doi.org/10.1590/S1516-14392009000100002>.
11. Amanda Dantas de Oliveira, Cesar Augusto Gonçalves Beatrice, (2018), Polymer Nanocomposites with Different Types of Nanofiller, DOI: 10.5772/intechopen.81329.
12. Maria Inês Bruno Tavares, Emerson Oliveira da Silva, Paulo Rangel Cruz da Silva and Livia Rodrigues de Menezes, (2017), Polymer Nanocomposites, DOI: 10.5772/intechopen.68142.
13. Dinesh Kumar S , Purushothaman S, (2016),Synthesis and Characterization of Polymer Nanocomposites for Biomedical Applications - Current Perspectives and Challenges,*International Journal of Research in Engineering and Science (IJRES) ISSN (Online): 2320-9364*.
14. Anindya Sarkar, Gautam Majumdar, (2022), Fabrication and Characterization of Flexible Semi-conducting Nanocomposite Polymer,*Sciencedirect.com*.
15. Ibrahim R. Agool, Kadhim J. Kadhim, Ahmed Hashim,(2017),Synthesis of (PVA–PEG–PVP–ZrO₂) nanocomposites for energy release and gamma shielding applications, DOI 10.1007/s12588-017-9196-1, research gate.
16. Cheng Hu , Jianxun Sun , Cheng Long , Lina Wu , Changchun Zhou and Xingdong Zhang,(2019),Synthesis of nano zirconium oxide and its application in dentistry,From the journal *Nanotechnology Reviews*, <https://doi.org/10.1515/ntrev-2019-0035>.
17. *Journal of Genetic and Environmental Resources Conservation* , 5(1):6-23, www.jgerc.com Print ISSN: 2306-8663, Online ISSN: 2306 – 8280.
18. S. Rajeshkumar, J.Santhoshkumar, Leta Tesfaye Jule, and Krishnaraj Ramaswamy, (2021), Phytosynthesis of Titanium Dioxide Nanoparticles Using King of Bitter *Andrographis paniculata* and Its Embryonic Toxicology Evaluation and Biomedical Potential, Hindawi, *Bioinorganic Chemistry and Applications*, Article ID 6267634, <https://doi.org/10.1155/2021/6267634>.
19. Liang Chu, Zhengfei Qin, JianpingYang,a, and Xing'ao Lib, (2015), Anatase TiO₂ Nanoparticles with Exposed {001} Facets for Efficient Dye-Sensitized Solar Cells, National library of medicine, doi: 10.1038/srep12143.

20. Nisha Elizabeth Sunny , Sneha Susan Mathew , Nandita Chandel , Panchamoorthy Saravanan, R. Rajeshkannan , M. Rajasimman , Yasser Vasseghian , N. Rajamohan , S. Venkat Kumar,(2022),Green synthesis of titanium dioxide nanoparticles using plant biomass and their applications- a review, Green synthesis of titanium dioxide nanoparticles using plant biomass and their applications- A review <https://doi.org/10.1016/j.chemosphere.2022.134612>