COMPARATIVE STUDY OF ALUMINIUM DOPED ZINC OXIDE FOR PHOTOVOLTAIC CELL

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RESEARCH COMPLETION CERTIFICATE

It is certified that Ms. Fatima Ejaz of BS (session 2019-2023), Department of Physics has carried out research work entitled **“Comparative study of Aluminium doped Zinc Oxide for Photovoltaic Cell”** under my supervision.
It is assured that research work is original and has not yet been published anywhere else.

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May Allah shower His blessings upon all of us. Ameen.

Fatima Ejaz

ABSTRACT

Energy is an essential component of our daily life, and it is hard to imagine a day without it. The photovoltaic cell produces voltage or electric current by utilizing sunlight through the photovoltaic effect. While silicon photovoltaic (PV) cells grown on wafers have the disadvantage of being expensive and low in efficiency, thin-film (PV) cells technology is utilized for efficient energy production. Photovoltaic devices extensively utilize Aluminium-doped Zinc oxide thin films (AZO) due to their functionality of light transmission. This study investigated the thin film deposition on soda lime, borosilicate, and simple looking glass substrates using the Aluminium doped ZnO technique and radio frequency magnetron (RF) sputtering method, with a focus on sputtering power (W) on the optical properties of the films and structural analysis of the film. X-ray diffraction abbreviated as XRD and an Ultraviolet visible spectroscopy have been used to explore and analyze the Aluminium doped zinc oxide thin films. The observed diffraction peaks in all the AZO thin films were found to exhibit a hexagonal wurtzite crystal structure, with a predominant growth orientation forward the (0 0 2) plane and the c-axis perpendicular to the substrate, as evaluated through structural analysis. Transmittance measurements were conducted to gain the desired optical properties of thin films. It was discovered that film thickness had a significant impact on the optical band gap, with the band gap of samples 1, 2, and 3 increasing with the sputtering power (W). The optical band gap of aluminium doped zinc oxide increased with increasing sputtering power in the range of 30 to 500 W. The increase in sputtering power resulted in an increase in film thickness, leading to higher optical transparency and a widening of the band gap.

COMPARATIVE STUDY OF ALUMINIUM DOPED ZINC OXIDE FOR PHOTOVOLTAIC CELL

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LIST OF ABBREVIATIONS

PV	Photovoltaic Cell
AZO	Aluminium doped Zinc Oxide
ZnO	Zinc Oxide
Al	Aluminium
RF	Radio Frequency
eV	Electron-volts
UV	Ultraviolet
LED	Light Emitting Diode
XRD	X-ray diffraction
Ar	Argon

UV-Vis	Ultraviolet visible
PSC	perovskite solar cell

CHAPTER 1

INTRODUCTION

1.1 Solar Energy

The most integral part of our everyday life is energy, and it is difficult to live a single day without energy. Our work is done by the use of energy. Energy gets converted from one form to another and in this process of energy conversion we get work done [1].

Solar energy refers to any energy derived from the sun, and it's the most abundant and sustainable energy source globally. The sun generates solar energy through nuclear fusion, which manifests as electromagnetic radiation in the form of heat and light. These waves exist at varying frequencies and wavelengths, with most of them invisible to the human eye. The waves with high-frequency emitted by sun, such as X-rays, gamma rays, and UV rays, are visible to us. Solar energy systems are technologies that transform the sun's heat or light into another form of energy that we can use [2].

Figure 1.1 the preservation of energy resources and the use of solar power [3].

1.2 Photovoltaic Effect

The photovoltaic cell is capable of producing voltage or electric current when exposed to sunlight through a process known as the photovoltaic effect. Photons which are comprised by sunlight are packets of energy that can be soak up by the photovoltaic cell. Specifically, when photons with the appropriate wavelength hit the p-n junction of the cell, they transfer energy to atoms in on semiconductor material, causing electrons (e^-) to move to a state with higher energy. The process generates an electron-hole pair, which acts as two charge carriers [4].

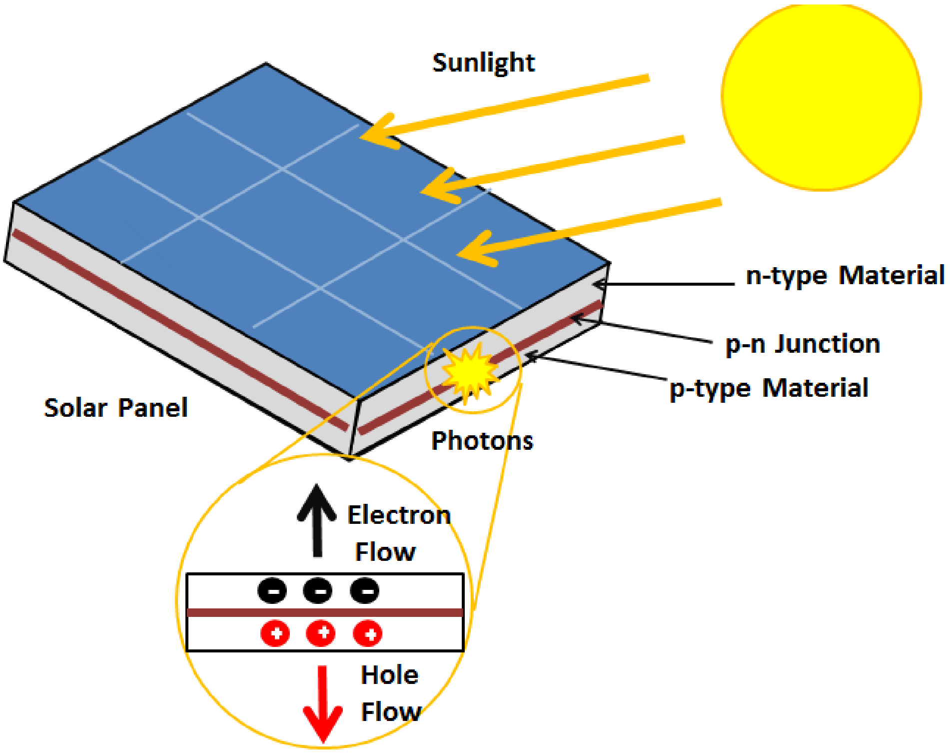

Figure 1.2 a diagram showing the photovoltaic effect [5].

Semiconducting matter holds electrons all together by generating the bonds with atoms when they are not present in an excited state of an atom. Consequently, the electrons (e^-) remain immobile. However, in the conduction band when they come to the excited state, they become freely to move. Electrons as well as holes proceed in the direction. The movement of electron (e^-) generates a current (I) within the cell. With the movement of electrons hole move in opposite direction. This process is responsible for the current produced by the cell [5].

1.3 Photovoltaic Cell

A technology that used energy from the sun and converts this energy into electricity is called a photovoltaic (PV) cell. This is achieved through a mechanism called the photovoltaic (PV) effect. Many photovoltaic cells exist; all used to interact with photons coming from the sunlight and produce current [5].

Figure 1.3 A solar panel, consisting of many photovoltaic cells [5].

Solar cells differ from batteries and fuel cells in that they do not rely on chemical reactions or fuel to generate electricity. They also lack any moving components, in contrast to electric generators. These cells can be organized into large groupings known as arrays, comprising thousands of individual photovoltaic cells [6].

1.4 History of Photovoltaic cell

1.4.1 Silicon Photovoltaic (PV) cells

In photovoltaic (PV) cells silicon is most commonly used. Currently, over 90% market comprises of photovoltaic (PV) cell made of silicon. Crystalline silicon made of crystal photovoltaic (PV) cells is silicon atoms connected to together to form lattice crystal. It provides an organized structure that makes conversion of light into electricity [4].

1.4.2 Thin film Photovoltaic (PV) cells

Thin film photovoltaic (PV) cells are another popular photovoltaic technology, characterized by their composition of thinner layers of material i.e. semiconductor. These layers are a few micro meter (m) thick. Their flexible nature renders them useful for mobile applications. Additionally, some thin film photovoltaic (PV) cells have producing techniques that require little energy and are more easily scalable than the techniques needed for silicon photovoltaic (PV) cells [7].

1.5 Difference between Thin-Film and Silicon PV Cells

- Silicon photovoltaic (PV) cells called first generation PV cells grown on wafer and of silicon. It has low efficiency as compared to thin films. Thin films (PV) cells called second generation of PV cell. This technology is used to produce electrical energy and efficiency of the photovoltaic (PV) cell increases.
- In earlier versions of thin film technology, silicon wafer was used in the conversion of sunlight into power (electrical). In photovoltaic (PV) technology, electron hole pair production is utilized.
- Silicon photovoltaic (PV) cells cover 80% of the solar panel but are less economical while on the other hand thin film photovoltaic (PV) cells are more economical and developed technology market.
- Traditional silicon photovoltaic (PV) cells have recorded high efficiencies, but their production requires pure silicon and energy-intensive processes, which makes them expensive compared to the output power they generate. In contrast, thin film photovoltaic (PV) cells require less energy, cost and precious time making them a preferred option for second-generation solar cells with a lower cost-to-output power ratio [8].

1.6 Structure and working of Thin Film PV Cell

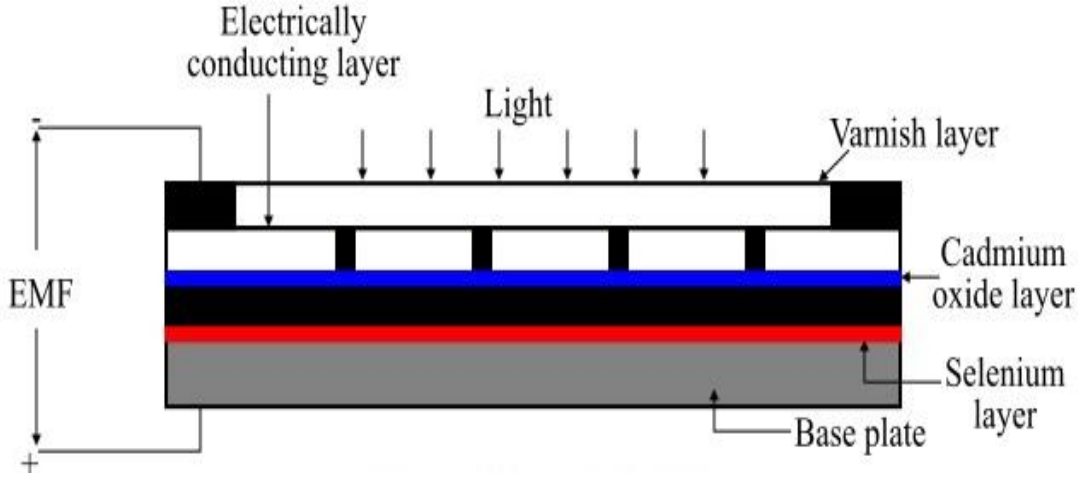

Figure 1.4 Construction of a photovoltaic cell [9].

A photovoltaic cell is composed of a metallic plate, typically made of aluminum, on which light-sensitive metallic layer is placed as the (+) terminal. A thinner layer which allows light to reach the selenium is then applied through sputtering, serving as the negative terminal. A strip of metal is sprayed on the top surface edge to create the negative contact. To protect the front surface of the photovoltaic cell, a transparent varnish layer is applied. When light hits the selenium layer through the cadmium oxide layer, the selenium compound releases electrons, which are sufficient to create a current flow through the external circuit connected between the positive and negative terminals [9].

1.7 Applications of Photovoltaic Cell

Some applications of photovoltaic (PV) cells are given below:

1.7.1 Photovoltaic cell for Transportation

Photovoltaic cells are utilized to create solar power, which is used in cars to power the motor or transferred to the storage battery. The first solar car was built by Ed Passerini. The utilization of solar energy in cars has become increasingly popular in recent years.

1.7.2 Photovoltaic cell in Calculators

Solar-powered calculators utilize photovoltaic cells to operate, drawing energy from the light of the sun. This means that they work solely with solar energy and are particularly effective in outdoor light.

1.7.3 Solar Cell Panels

Solar panels are installed on the rooftop to serve multiple purposes. Firstly, they function as a solar heater, utilizing the sun's energy to heat water that can be used for bathing. In addition, they are able to generate power, which can be stored in a backup battery and used during power outages. Alternatively, this energy can be stored and used to generate electricity in the home, leading to reduced electricity bills and increased savings.

1.7.4 Solar Farms

A vast expanse of photovoltaic (PV) panels has the ability to generate power of utility-scale. The sizable systems are capable of supplying electricity to municipal or regional grids.

1.7.5 Stand-Alone Power

Photovoltaic (PV) technology is suitable for powering stand-alone devices, tools, and meters in both urban and remote areas. PV systems can provide electricity to a variety of applications.

1.7.6 Power in Space

Photovoltaic (PV) technology has served as a power for orbiting satellites from its inception. The utilization of higher capability PV has facilitated power supply for ambitious projects. PV is set to an essential component of space in the future [10].

1.8 Band Gap of Photovoltaic Cells

Energy difference of the band gap is minimum connecting top and bottom of valence and conduction band. In a band gap i.e. direct, top and bottom of valence and conduction band are situated at similar value (k). Conversely, in a band gap i.e. indirect, top and bottom of valence and conduction band are situated at different value (k). This distinction is particularly significant in optoelectronic devices.

Band gap i.e. direct, such as gallium arsenide are preferred for producing optical instrument such as LEDs and semiconductor lasers, while indirect band gap semiconductors like silicon are not [11].

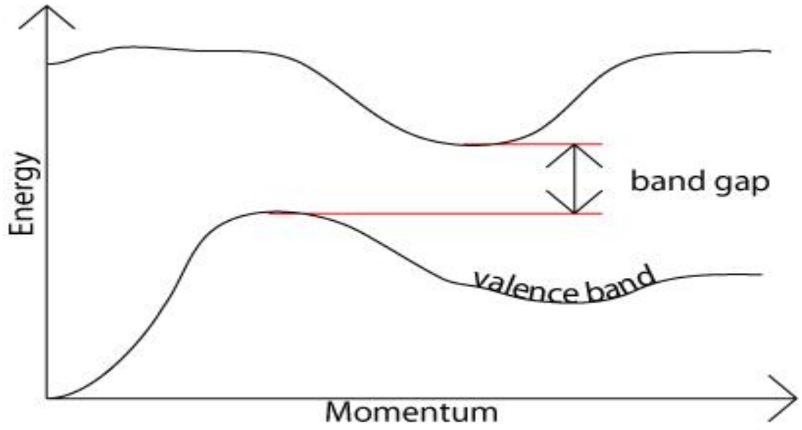

Figure 1.5 Direct and Indirect band gap of a semiconductor [11].

1.8.1 Uv-vis spectroscopy for optical band gap

UV-Vis spectroscopy is a technique that measures light absorption as a function of wavelength, providing insight into the electronic transitions taking place in a semiconductor material in response to incident light. This method is utilized to estimate the optical band gap [11].

1.9 Zinc Oxide as potential material for PV Cells

ZnO is an extinct compound. It is a colorless powder that does not dissolve in water. ZnO is incorporated into a wide range of materials and products as an additive [12].

Figure 1.6 Zinc Oxide (ZnO) nanoparticles [12].

ZnO has gained attention as a candidate for (TCO) applications in recent years, owing to its exceptional properties. These include good translucency over the visible and near-IR light range, a broad band gap exceeding 3.2 eV. Moreover, its massive availability of zinc makes it a cost-effective alternative for TCO applications. ZnO thin films doped with Aluminium gives optical transmittance, making them ideal for optoelectronic device i.e. PV cell applications [13].

$$Zn^{2+}O^{2-}$$

Figure 1.7 ZnO formula [12].

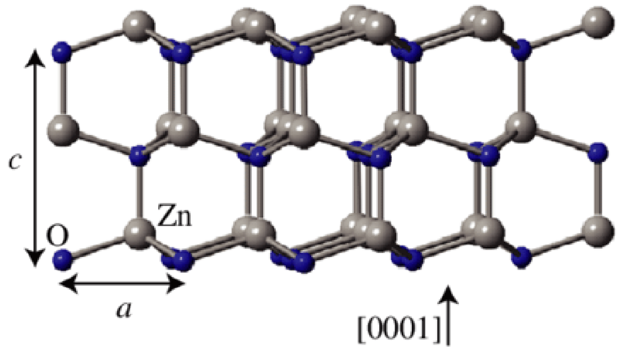

Figure 1.8 Wurtzite crystal structure of ZnO with lattice parameters a and c [12].

1.10 Aluminium; transition metal

Aluminium, represented by the chemical symbol Al has density approximately one-third that of steel and is lighter than other frequently used metals. Upon exposure to air, it readily reacts with oxygen to create an oxide layer on its surface. Aluminium has a reflective, silver-like appearance, and it is not magnetic. Additionally, it is flexible, bendable, and ductile [14].

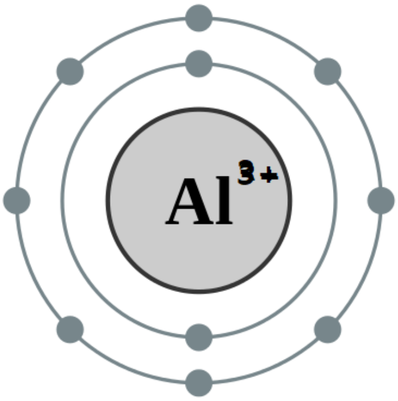

Figure 1.9 Atomic Structure of Al [15].

AZO has shown the lower resistivity (2 × 10^−5 Ω cm), making it a top contender to replace ITO. Several reports exist where doped ZnO was utilized in optoelectronic applications [16].

1.11 Doping

In the production of semiconductors, doping involves deliberately introducing impurities. It modifies optical and structural properties, resulting in the formation of an external semiconductor. When the amount of dopant added i.e. 100 million atoms, it is considered low doping. On the other hand, high doping occurs when dopant atoms are added more [17].

1.11.1 Effects on band structure

When a crystal structure is doped, band gap was institute with new energy states. These states are located closely to the energy band. For instance, (e^-) donor and acceptor impurities lead to the creation of states near the conduction band and valence band [17].

1.12 Radio Frequency (RF) Sputtering Method

In recent years, several methods have been employed for depositing thin films by AZO. Among these methods, RF magnetron sputtering has become widely used technology for producing thin films by AZO for photovoltaic (PV) cell applications. This is because it allows for good control of higher thickness over a large surface area.

RF sputtering is a thin-film deposition approach commonly used in the computer industries. Sputtering involves creating positive ions by passing a wave of energy through an inert argon (Ar) gas. However, there are differences between RF sputtering and direct current sputtering in terms of pressure and ideal target material [18].

RATIONALE

Solar industry has made significant strides in recent years, with numerous advancements in solar technology. These breakthroughs include photovoltaic cells with longer lifetimes, solar cells that can be applied to flexible surfaces, solar panels helps in the detecting of movement of sun and in the night solar power plants operates. One of the promising next-generation photovoltaic cells is the hybrid metal halide perovskite solar cell (PSC), which has garnered considerable attention due to its affordability, thicker design and light absorption properties, resulting in better performance under diffuse light conditions. Another promising technology is second-generation thin-film photovoltaic cells, which feature a narrow design with light-absorbing layers 350 times smaller than those found in standard Si-panels. These cells are lightweight, flexible, very easy to install, and hold significant promise for the future of the Nano Industry. This research aims to improve the performance of photovoltaic cells to meet future demands.

OBJECTIVES

Following are the objectives of this study:

- To study comparative analysis of Al doped ZnO for Photovoltaic Cells via Radio Frequency Magnetron Sputtering method.
- To study the structural analysis of thin films AZO by XRD technique.
- To investigate the optical effects of Al doped ZnO to serve as potential substance for photo voltaic cells.
- This study is to evaluate the tuning of optical band gap with the variation in Radio frequency magnetron sputtering power in the range 30- 500W.

CHAPTER 2

LITERATURE REVIEW

In a recent study by Chunhu Zhao et al. (2021), thin films Aluminum doped ZnO were investigated for their ability to transmitting the light, making them highly desirable for use in (PV) devices. To gain higher performance of films by AZO, the impact of radio frequency sputtering states on the optical properties of the thin films was determined. The thin films demonstrated a hexagonal wurtzite structure with a strong orientation along the (002) plane. At the optimal deposition condition of 120 W, an average transmittance of over 85% was achieved. These results suggest that radio frequency magnetron sputtering by AZO thin films hold great promise for use in photovoltaic cell applications [19].

In their study, Houda Ennacer et al. (2021) conducted experimental analyses on thin films of aluminum-doped zinc oxide (AZO) and zinc oxide (ZnO) prepared via radio frequency magnetron sputtering. The researchers analyzed the films' structural and optical properties and found that AZO thin films had higher optical transmittance compared to ZnO films of the same thickness. XRD analysis revealed a shift in growth orientation from vertical along the (002) crystallographic plane to lateral along the (103) plane with aluminum doping. The team also determined the optical properties of the ZnO and AZO films and observed that the optical band gap shifted to 3.34eV with aluminum doping [20].

Nader Ghobadi's et al. (2021) described, RF technique, by AZO on thin films. The impact of sputtering power on the films, optical characteristics was determined. Ultra-violet visible spectroscopy was used to find optical properties, which revealed that all AZO thin films had direct allowed transitions. Additionally, various physical quantities were reported for the AZO at different sputtering times (t). Method named Derivation Ineffective Thickness (DITM) Method was utilized to determine the band gap i.e. optical. The performance time was discovered to be an important factor in regulating the thin films' physical properties, helping to achieve the optimum thickness [21].

Woo-Lim Jeong et al. (2021) explained that transparent electrodes are typically considered a compromise between transmittance and the impact of thin-film interference on optoelectronic devices. This study examines the performance of solar cells using an AZO electrode which was transparent. The author distinguishes the transmittance (%) of the Aluminium doped Zinc Oxide electrode in the overall wavelength (450-800 nm) from the transmittance (551-700 nm) range for solar cells. The conclusion was made that a wide AZO transparent electrode has higher transmittance (87.2%) than a narrower AZO transparent electrode (82.8%) in the maximum absorption range. When applied to solar cells, the electrodes resulted in up to a 26% difference in power conversion efficiency. These results could be beneficial in improving the performance or adjusting the thin-film photovoltaic cells [22].

In their work, Young-He Jo et al. (2021) focused on Al-doped ZnO (AZO) as a transparent material electrode due to its little cost, higher transmittance, excellent mechanical flexibility and higher electrical conductivity. The authors explore the etching of Aluminium doped ZnO thin films in a BCl3/Ar-based plasma operator. Through optical emission, he revealed that the interaction between Ar ion bombardment and Cl1 and Cl2 radicals is responsible for the etching mechanism. The use of BCl3- plasma etching induced changes in the properties of the AZO surface, including increased smoothness, a 200 meV increase in work (W) function, and 0.03 eV increase in bandgap after the etching process [23].

Fatiha Challali et al. (2020) conducted a study on the deposition of thin films on glass substrate by AZO technique using the (RF) magnetron sputtering method at (RT) in confocal configuration. They utilized several techniques to analyze the effects of power, ranging from 50-350 W, on the structural properties and optical properties. The results revealed that the crystalline structure quality of AZO films was significantly affected by sputtering power, with an orientation along c-axis being obtained at lower sputtering power of 40 W. Using UV-Vis-NIR spectroscopy at room temperature the researchers found that the optical transmittance of the AZO thin films in the visible range (300-850 nm) was greater than 75% [24].

Hongyan Liu et al. (2020) investigated the impact of the columnar structure on the optical properties of thin films (AZO) deposited in-situ using the RF magnetron sputtering method. The sputtering power was varied from 130 W to 250 W, and the sample was obtained at 210 W (for 30 min), exhibiting an average transmittance of 83.2%. Cross section revealed that the columnar structure appeared at higher radio frequency power. However, the thickness at which it began to appear did not remain constant. Moreover, higher RF power resulted in a reduction of thickness. The Drude's model was used to investigate the relationship between optical properties and power. Based on XRD, the appearance of Al_2O_3 was found to significantly deteriorate the optical properties at 250 W [25].

In their study, Dipak Barman et al. (2020) aimed to fabricate thin films using interfaces of Ag nanoparticles and (AZO) deposited by radio frequency magnetron sputtering. The process was completed within 25-30 minutes without breaking the vacuum; preventing post-fabrication oxidation of Ag. High transmittance in AZO thin films with thickness below 2 hundred nm was achieved. The composite structure's figure of merit peaked at 40 mΩ-1 when Ag NPs were grown for almost 5 min. The fabrication of AZO interfaces in vacuum environment facilitated bending stability required for a transparent conductor [26].

Naveen Kumar et al. (2020) investigated a method to improve the AZO conductivity of thin film using a ZnO layer made of seed assisted sputtered deposition approach. The AZO thin film grown with the layer of seed exhibited excellent optoelectronic properties, with high optical transmittance (>90% in the Vis-NIR range). These characteristics make thin film by AZO suitable for applications include transparent electrode. The use of Nano scale Kelvin probe force microscopy revealed shorter boundary potential in the layer of seed, which was attributed to defects segregation towards grain boundaries. X-ray photo electron analysis confirmed the low carrier concentration, such as zinc and oxygen vacancies, in the AZO thin film with the layer of seed. Furthermore, the study of the defect chemistry and their Nano scale distribution showed that defects at grain border [27].

In this study, Pankaj K. Bhujbal et al. (2020) grew thin films AZO using RF magnetron sputtering at deposition temperature. The impact of temperature on the structural and optical properties of the films was investigated. Results from XRD revealed that AZO layers had a hexagonal crystal wurtzite structure with orientation along c-axis (002). The optical properties showed that the optical band gap energy was affected by the temperature in the substrate. By varying the deposition temperature from 22 to 400 ℃, transparent thin films with band gap ranging from 3.49 to 3.66 eV were achieved. Photoluminescence (PL) spectra confirmed the presence of defects [28].

Eugen Stamate et al. (2020) provided an explanation for the use of thin films based on AZO, which is considered as an alternative for little cost and large surface area applications like photovoltaic (PV) cells. Though significant research, there is still debate surrounding the films growth by RF magnetron sputtering, particularly with regard to the role of oxygen (O) negative ions. This study shows a method for reducing thin film resistivity by over 2 times. This electrode increases coupling of radio frequency magnetron sputtering and improves electronic properties Thus the resistivity below 3 × 10^−4 Ωcm is achieved over a substrate with the surface, without any intentional substrate heating, while maintaining an averaged transmittance above 90% [29].

Michel Chaves et al. (2019) conducted a study on the synthesis of thin films on glass substrates by AZO using radio frequency (rf) magnetron sputtering from a metallic Zn-Al (5.0 at. %). The effects of radio frequency sputtering pressure, which varied from 0.2 to 6.8 Pa, on the structural properties and optical properties of the thin films were investigated. (XRD) analysis revealed that the thin films were polycrystalline, had a wurtzite hexagonal structure, and an orientation preferential in the (002) plane. The crystallite size of the films is increasing with increasing sputtering pressure. The results showed that the structure zone alone could not determine the structural properties of the AZO thin films. The methodology used in it was allowed for the deposition of transparent conductive electrodes [30].

Hongyan Liu et al. (2019) conducted a study to improve the properties of thin films AZO by optimizing the deposition process. The thin films were fabricated on substrates made of glass at room temperature using (RF) magnetron sputtering with fluctuating Argon (Ar) flow rates ranging from 36 to 68 sccm. The effects of Argon

(Ar) flowing rate on the structural, morphological, photoluminescence and optical properties of the AZO thin films were determined. The highest quality AZO film, which had an average visible transmittance of 84.2%, was produced by depositing the film at 44.0 sccm for 0.5 seconds. The researchers also examined the self-heating effect of the target by depositing AZO [31].

G. Tong et al. (2019) demonstrated a method for enhancing the properties of thin films AZO by treating them with hydrogen (H2) plasma for varying durations following radio frequency magnetron sputtering at RT. The results showed that at conditions of 10.0 W, 200 °C, and 3 hours, the transmittance of thin films improved from 90.5% to 96.0% at a wavelength of 550 nm. The optical characteristics of the hydrogen plasma-treated thin films were analyzed using a spectroscopic ellipsometer, and the results indicated a decline in the refractive index (n) throughout the wavelength (µ) range of 351-1100 nm. Above findings could be useful in the development and optimization of optoelectronic applications based on AZO thin film [32].

Pankaj K. Bhujbal et al. (2019) have reported on the successful growth of clear and conducting thin films AZO using the RF sputtering technique. XRD data indicated that the substrate deposited at low radio frequency power (100 Watt) was amorphous, while the thin film deposited at 200 Watt radio frequency power showed the c-axis (002) preferential orientation and exhibited a wurtzite crystal of hexagonal structure. Optical analysis determined that the crystalline thin film had a greater average roughness and thickness compared to the amorphous thin film. The optical band gap decreases and the crystalline sample were attributed to the increase in thickness and crystallite size as a result of confinement effect [33].

Chuanhe Ma et al. (2018) explained the impact of different sputtering parameters i.e. power, pressure and temperature on the optical transmittance (%) of thin films AZO deposited using sputtering i.e. radio frequency sputtering. The results showed in the experiment is that optical transmittance remained almost unchanged. Through optimizing the parameters to 0.4 Pa, 200°C, 125 minutes, and 180 W, using an AZO target with 2wt% Al_2O_3, high-quality AZO thin films with over 84% transmittance and a thickness of 1500 nm were produced. These optimized parameters were also used to grow a thin-film PV cell [34].

Ke Cheng et al. (2017) conducted research on the use of AZO thin films as a transparent conducting oxide for photovoltaic (PV) applications. They employed radio frequency (RF) magnetron sputtering to deposit AZO films on glass substrates and examined the effect of substrate temperatures on the films' structural and optical properties. The results indicated that all AZO films possessed a hexagonal structure with a preferred orientation along the c-axis. The films were highly transparent from the ultraviolet to near-infrared range, with an average transparency exceeding 83%. The practicality of the AZO film as a transparent electrode in a Cu(In1-xGax)Se2 (CIGS) photovoltaic device was also evaluated. Thanks to the high transparency and conductivity of the AZO film, the efficient device demonstrated an efficiency of 7.8%, with a short-circuit current density of 28.99 mA/cm2, an open-circuit voltage of 430 mV, and a fill factor of 62.44 under standard conditions [45].

Yi-hua SUN et al. (2016) conducted a study on the deposition of Aluminum-doped zinc oxide (AZO) thin films on glass substrates using RF magnetron sputtering at room temperature. The researchers examined the microstructure and optical properties of the AZO thin films using X-ray diffraction and UV-visible spectrophotometry. The findings indicated that all films were polycrystalline and exhibited a hexagonal structure, with an average optical transmittance exceeding 85% at various sputtering powers. The optical band gap of the films was found to range between 3.48 and 3.68 Ev [36].

H. Dondapati et al. (2013) conducted a study on the growth of aluminum-doped ZnO thin films on glass substrates using rf-magnetron sputtering. Their findings showed that increasing the substrate temperature can improve the crystallinity of the ZnO thin films, as determined by XRD analysis. The researchers obtained AZO samples grown at 450C with over 85% transmittance. They attributed the low resistivity and high transmittance to the combination of dopant and oxygen vacancy concentration. The authors suggested that the high optical transmittance of AZO films holds great potential for their application in flexible electronic devices, such as transparent conducting oxide film on LEDs, solar cells, and touch panels [37].

CHAPTER 3

METHODOLOGY

3.1 Sample preparation via RF Sputtering technique

The deposition of AZO thin films onto glass substrates by RF magnetron sputtering was carried out, using Ar gas as the sputtering gas. The glass substrates were thoroughly cleaned and dried with nitrogen gas prior to deposition. The vacuum chamber was pumped down to a base pressure using a molecular pump. Sputtering power in the range of 30-500 W was applied to the target, and a pre-sputtering step was performed to eliminate surface contamination of the target. X-ray diffraction analysis was used to determine the crystal structure of the AZO thin films. The band gap was obtained from optical transmittance data collected at room temperature [19, 24 38].

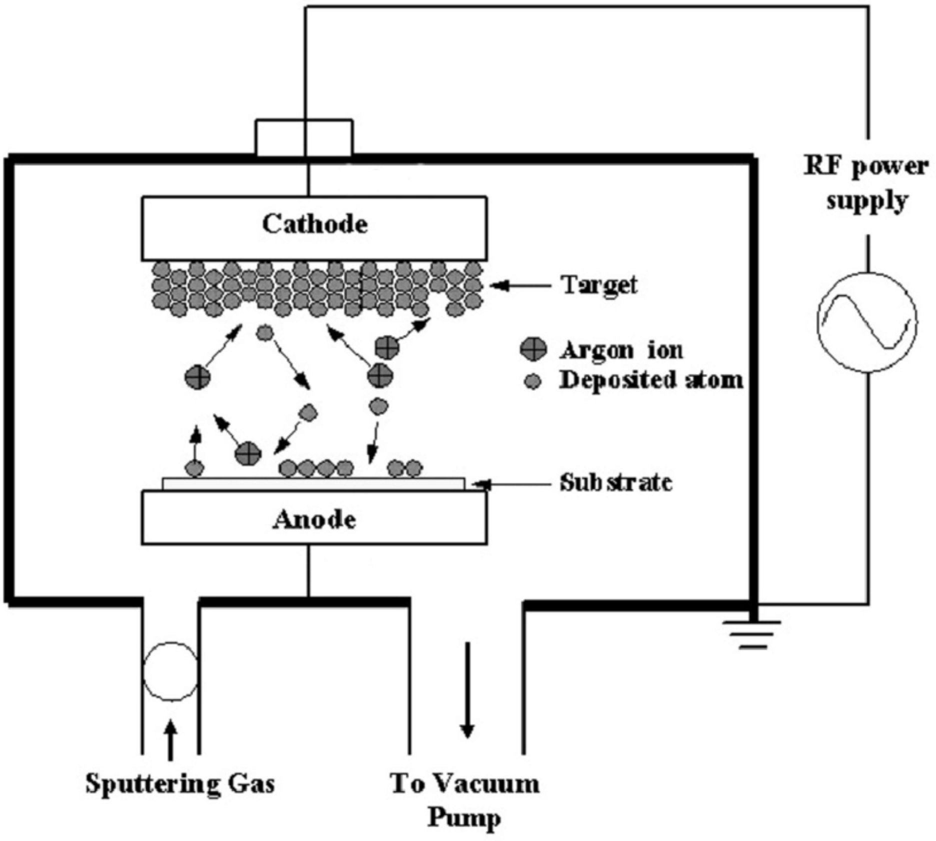

Figure 3.1 RF Sputtering System Schematic Diagram [31]

Table 3.1 Parameters and Specifications of Sample 1, 2 and 3 [9,24,38].

S.N		Sample 1	Sample 2	Sample 3
	Specifications:			

1.	Glass Substrate	Soda lime glass substrates	Borosilicate glass substrates	Simple glass substrates
2.	Diameter	50mm	2-inch	60mm
3.	Base pressure	5*10^-4 Pa	2×10^-5 Pa	2.3×10^−3 Pa
4.	Working pressure	0.2–1.0 Pascal	0.6 Pascal	0.5 Pascal
5.	Sputtering power	30-120W	50-300W	200-500W
6.	Film thickness	---	115-180nm	500nm
7.	Distance	65mm	12mm	55mm
8.	Deposition time	45 min	1 hour	20 min
9.	Mass ratio	2:98	---	---
10.	Components	ZnO:Al2O3	ZnO:Al2O3	Al2O3
11.	Concentration	---	98:2wt.%	2%

Table 3.2 Process gas apply in sample 1, 2 and 3 [9,24,38].

S.N		**Sample 1**	**Sample 2**	**Sample 3**
	Process gas apply:			
1.	Gas	Argon	Argon	Argon
2.	Flow	30 sccm	20 sccm	20 mL/min
3.	Purity	99.999%	99.99%	99.99 %
4.	Cleaning agent	Ethanol, acetone and distilled water	acetone, methanol, and deionized water	Ethanol, acetone and distilled water
5.	Drying agent	Nitrogen	Nitrogen	---

3.2 Techniques for the characterization

3.2.1 X-ray diffraction (XRD) for structural analysis

X-ray diffraction analysis, also known as XRD, is a technique in materials science that is utilized to ascertain the crystallographic structure of a material. This method involves exposing a material to X-rays and then measuring the intensities and scattering angles of the X-rays that emerge from the substance. One of the most common applications of XRD analysis is the identification of materials by analyzing their diffraction patterns. Apart from identifying phases, XRD also provides information on the differences between the actual and ideal structure due to internal stresses and defects. XRD is a non-destructive technique that has many advantages and applications, such as identifying crystalline phases and orientation, as well as determining structural properties [40].

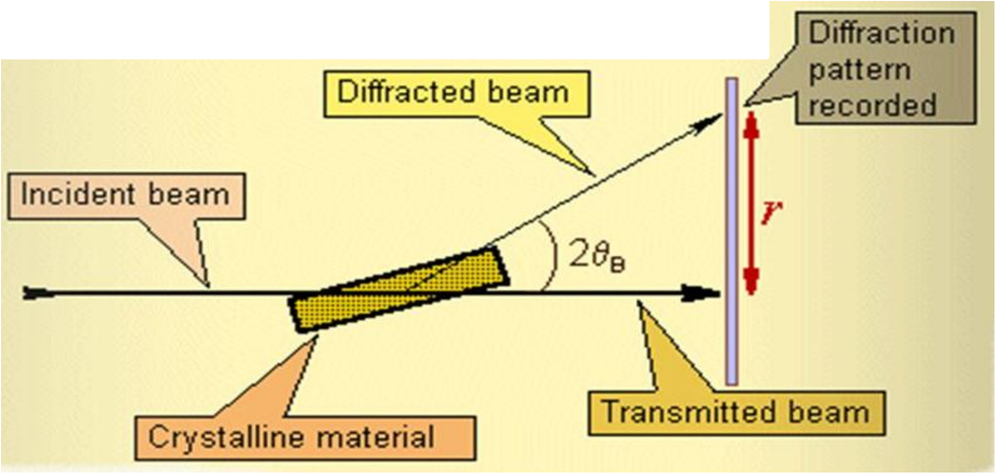

Figure 3.3 Detailed diagram of XRD [40].

3.2.2 Ultraviolet-visible (UV-Vis) spectrophotometry for optical analysis

UV-visible (UV-Vis) spectrophotometry is a technique utilized to quantify the optical absorption of a material in the ultraviolet and visible regions of the electromagnetic spectrum. The medium through which light passes can absorb, reflect or transmit the incident light. Absorption of UV-visible light results in atomic excitation, which is a phenomenon where molecules transition from a low or ground state to an excited state [39].

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Structural Analysis of sample 1, 2 and 3 via XRD

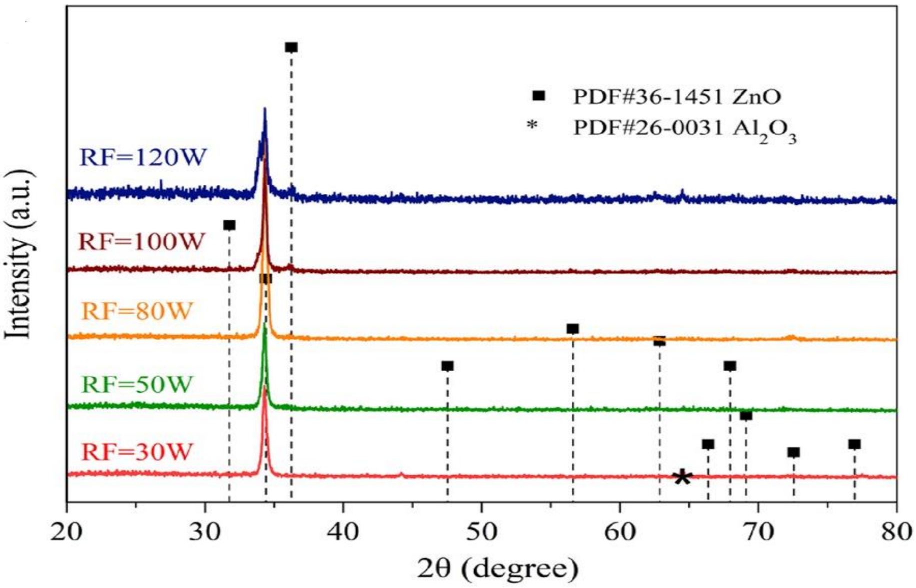

Figure 4.1 patterns through XRD technique of the thin films with RF (magnetron sputtering) sputtering power i.e. 30, 50, 80, 100, and 120 W, respectively [9].

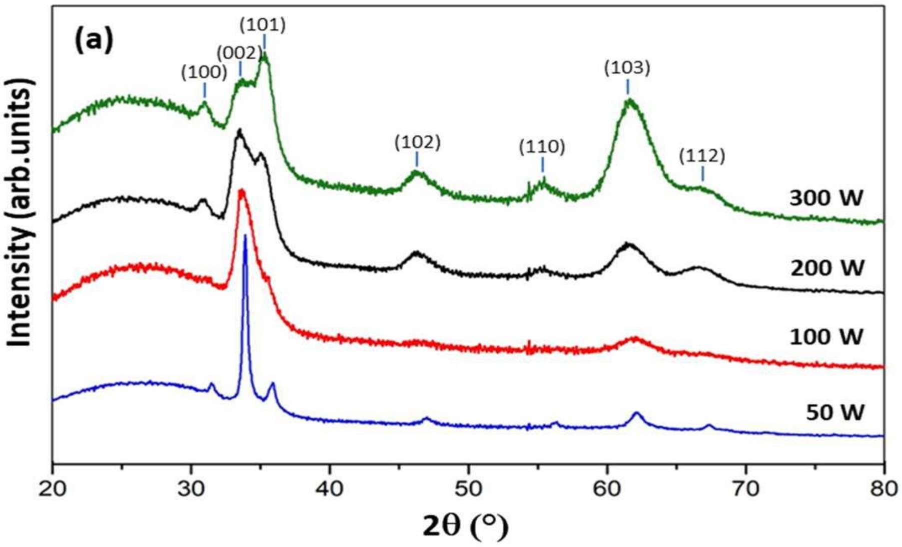

Figure 4.2 patterns through XRD technique of the thin films with RF (magnetron sputtering) sputtering power i.e. 50, 100, 200 and 300 W respectively [24].

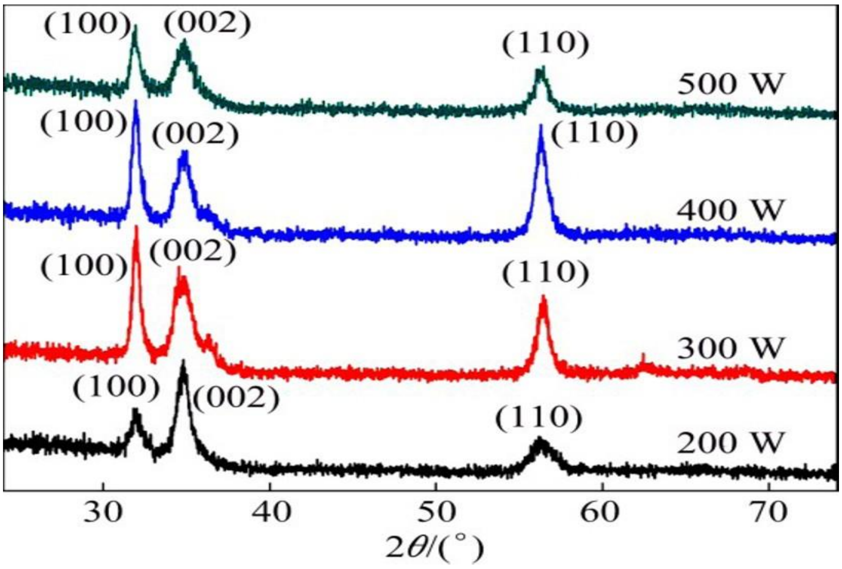

Fig. 4.3 patterns through XRD technique of the thin films with RF (magnetron sputtering) sputtering power i.e. 200, 300, 400 and 500 W respectively [38]

4.1.1 Sample 1

- The XRD analyses were performed on all AZO thin films using soda lime glass substrates.
- Figure 4.1 illustrates Bragg's angle (2θ) and Intensity (a.u) graph of the thin films.
- The XRD patterns of AZO thin films deposited at various RF sputtering power are presented in the figure.
- The diffraction peaks of the AZO thin films in Figure 4.1 correspond well with the standard XRD pattern of zinc oxide (PDF#36-1451), indicating the formation of a hexagonal wurtzite crystal structure.
- ZnO thin films sputtered onto a substrate show preferential growth perpendicular to the substrate, which results in highly textured films [9].

4.1.2 Sample 2

- Figure 4.2 is between Bragg's angle (2θ) and Intensity (arb. units) graph of the thin films.
- Figure 4.2 illustrates the GIXRD patterns of AZO thin films grown on borosilicate glass substrates at different RF sputtering powers.

- All the AZO films exhibit diffraction peaks that are significant for hexagonal wurtzite structure and are crystallized at (002) peak along c axis [25].

4.1.3 Sample 3

- Fig. 4.3 presents XRD patterns of films deposited on glass substrate at room temperature by RF sputtering.
- The observed diffraction peaks in all AZO thin films match with the diffraction of the hexagonal wurtzite structure of ZnO, such as (1 0 0), (0 0 2), and (1 1 0).
- The preference for growth orientation perpendicular to the substrate is indicated by AZO thin films growing along the (0 0 2) plane, showing that the c-axis is predominantly preferred for growth orientation.
- The (0 0 2) peak exhibits the intensity at 200 W among all sputtering powers [30].

4.2 Optical Analysis of sample 1, 2 and 3 via UV-Vis Spectroscopy

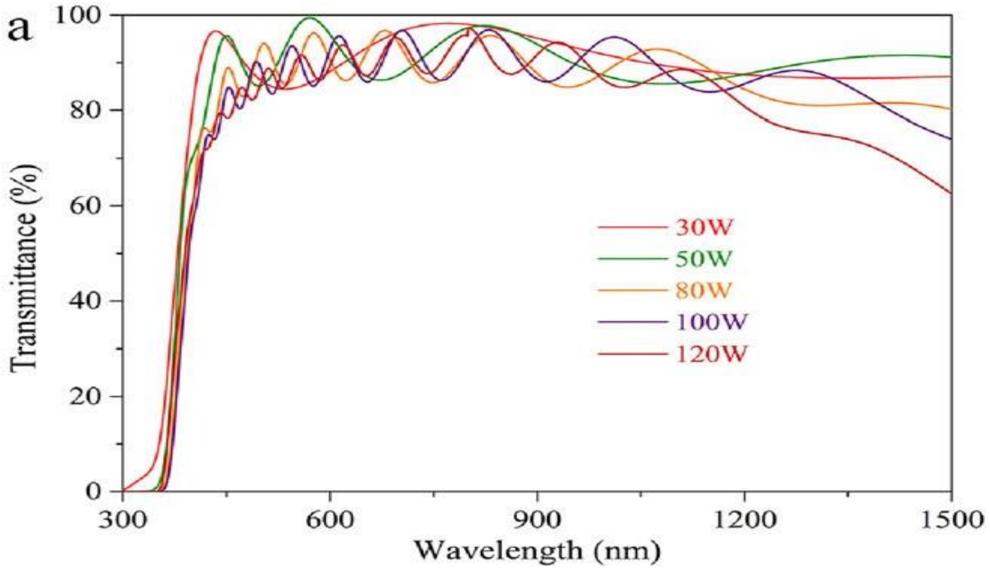

Figure 4.4 Transmittance (%) of optical properties of thin films at 30, 50, 80, 100 and 120 W sputtering powers [9].

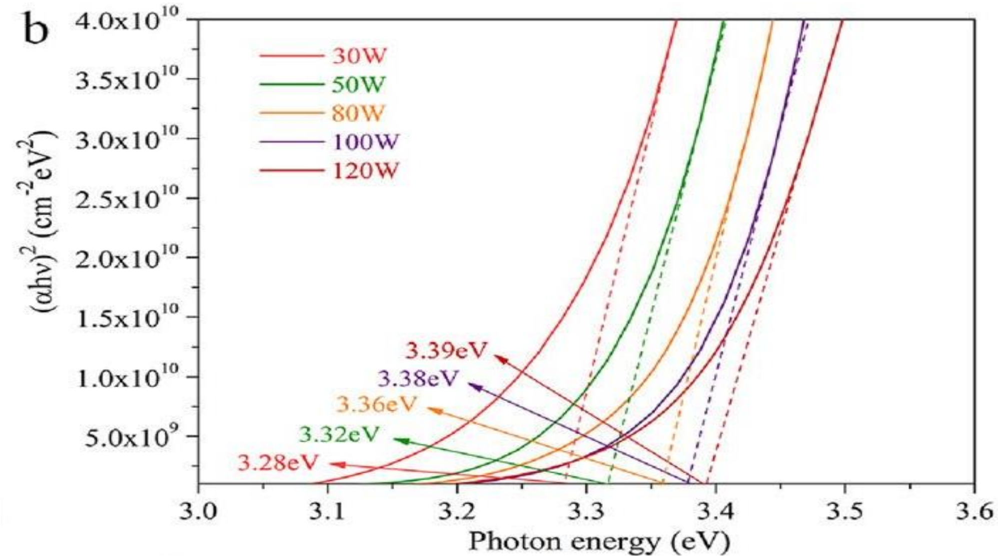

Figure 4.5 Band gap (eV) of optical properties of thin films at 30, 50, 80, 100 and 120 W sputtering powers [9].

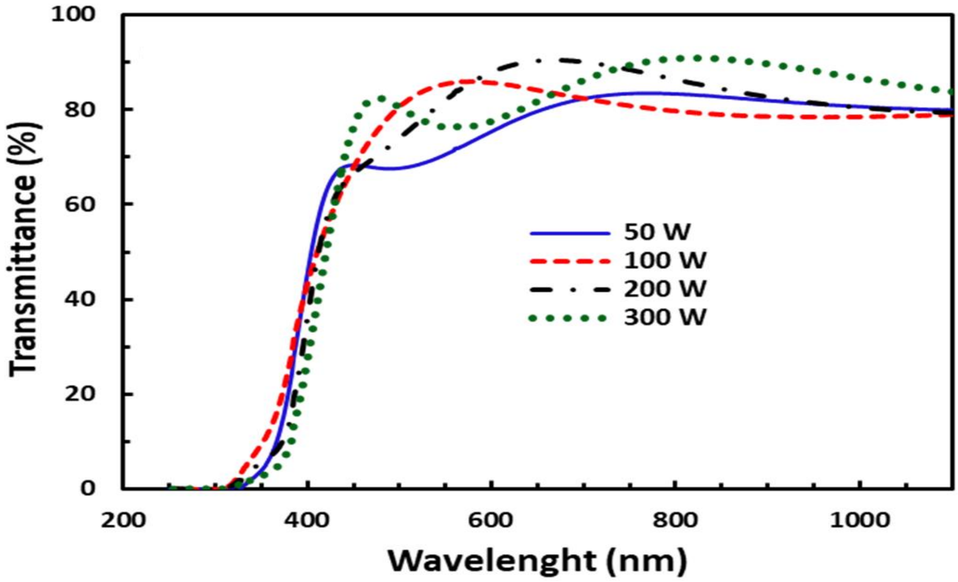

Figure 4.6 Transmittance (%) of optical properties of thin films at 50, 100, 200 and 300 W sputtering powers [25].

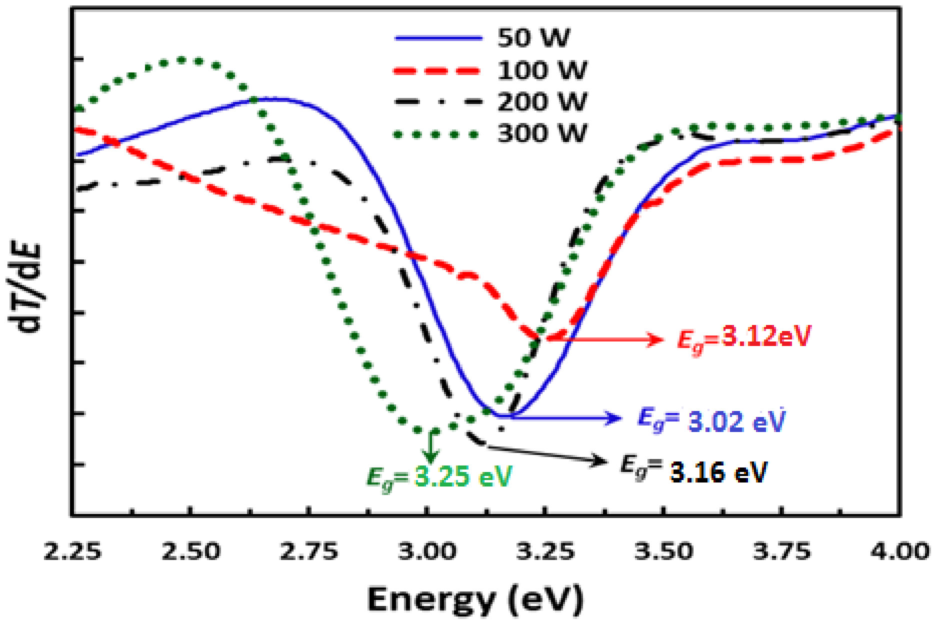

Figure 4.7 Band gap (eV) of optical properties of thin films at 50, 100, 200 and 300 W sputtering powers [25].

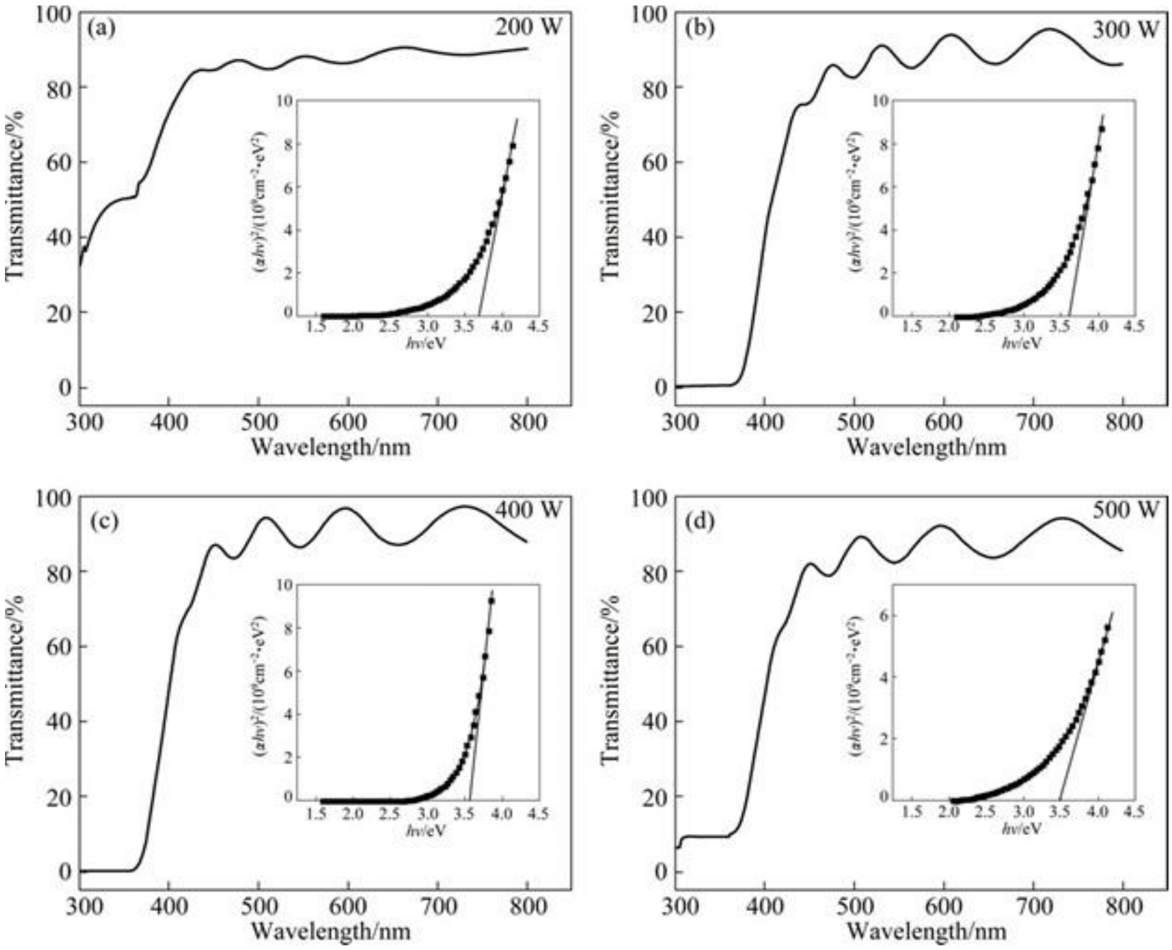

Figure 4.8 Transmittance and band gap spectra for AZO in a,b,c and d [38].

4.2.1 Sample 1

- Measurement of transmittance was performed on to optical properties for AZO thin films.
- The films are highly transparent within the 400-1100 nm range, with an average transmittance of up to 85%.
- Interference fringes pattern visible in spectra of as-deposited films varies with film thickness.
- Film thickness has a significant impact on it.
- The absorption coefficient (α) of AZO thin films can be calculated using $T=\exp(-\alpha d)$ based on their optical transmittance (T).
- (E_g) of AZO thin films can be determined using linear extrapolation of $(\alpha h\nu)^2$ plot with incident photon energy ($h\nu$) for direct transition.

- The optical band gaps of AZO thin films deposited at different RF sputtering powers were determined using the above calculation method.
- Figure 4.5 presents the results, which show that the band gap of the films increased from 3.29 to 3.40 eV with the increase of RF sputtering power [9].

4.4.2 Sample 2

- The transmittance of films with respect to air was measured using a UV-Vis-NIR spectrophotometer.
- The readings were conducted in µ range of 250 to 1100 nm to examine the impact of RF power on the films.
- The results are presented in Figure 4.6.
- The transmittance of films across all samples was 75-81% within the visible range of 400-800 nm, indicating a modest effect of sputtering power
- The technique used to determine the direct optical band gap (Eg) of AZO thin films is the first derivative of transmittance (dT/dE) as a function of energy (E).
- The data source used in this technique is transmittance spectra.
- Figure 4.7 shows dT/dE as a function of E for deposited AZO thin films vs RF power.
- The trend observed in the figure is that the band gap increases with increasing sputtering power [28].

4.4.3 Sample 3

- Figure 4.8 Optical transmittances of films deposited at room temperature with different sputtering powers in the wavelength range of 300-800 nm.
- All AZO thin films had a transmittance of more than 85% within the visible light range of 450-800 nm.
- The AZO thin film with the highest optical transmittance (89%) was observed at a sputtering power of 400 W.
- For the direct transition, the relation between (α) and (hν) can be given as: $(\alpha h\nu)^2 = A(h\nu - Eg)$.

- From the intercepts on the hν axis, the optical band gaps of thin films deposited at different sputtering powers are 3.48, 3.57, 3.62, and 3.68 eV.
- The widening of optical band gap was moderated as the sputtering power increased, and the values of band gap were increasing [38].

Table 4.1 AZO thin films optical properties w.r.t sample 1 [9]

Sputtering Power (W)	Substrate temperature (° C)	Transmittance (%)	Band gap (eV)
30	Room temp.	92.54	3.28
50	Room temp.	90.71	3.32
80	Room temp.	89.08	3.36
100	Room temp.	88.90	3.38
120	Room temp.	83.92	3.39
120	150	88.10	3.43
120	200	85.76	3.52

Table 4.2 AZO thin films optical properties w.r.t sample 2 [25]

Sputtering Power (W)	Substrate temperature (° C)	Transmittance (%)	Band gap (eV)
50	-	75	3.16
50	200	78	3.27
50	400	86	3.02
100	-	79	3.12
200	-	81	3.25
300	-	79	3.33

Table 4.3 AZO thin films optical properties w.r.t sample 3 [38]

Sputtering Power (W)	Substrate temperature (° C)	Transmittance (%)	Band gap (eV)
200	RT	87	3.48
300	RT	above 85	3.57
400	RT	89	3.62
500	RT	Above 85	3.68

Table 4.4 Tuning of Optical Bandgap for AZO films with sputtering power [9,24,38]

Sample 1		Sample 2		Sample 3	
Sputtering Power (W)	**Band gap (eV)**	**Sputtering Power (W)**	**Band gap (eV)**	**Sputtering Power (W)**	**Band gap (eV)**
30	3.28	50	3.02	200	3.48
50	3.32	100	3.12	300	3.57
80	3.36	200	3.25	400	3.62
100	3.38	300	3.33	500	3.68

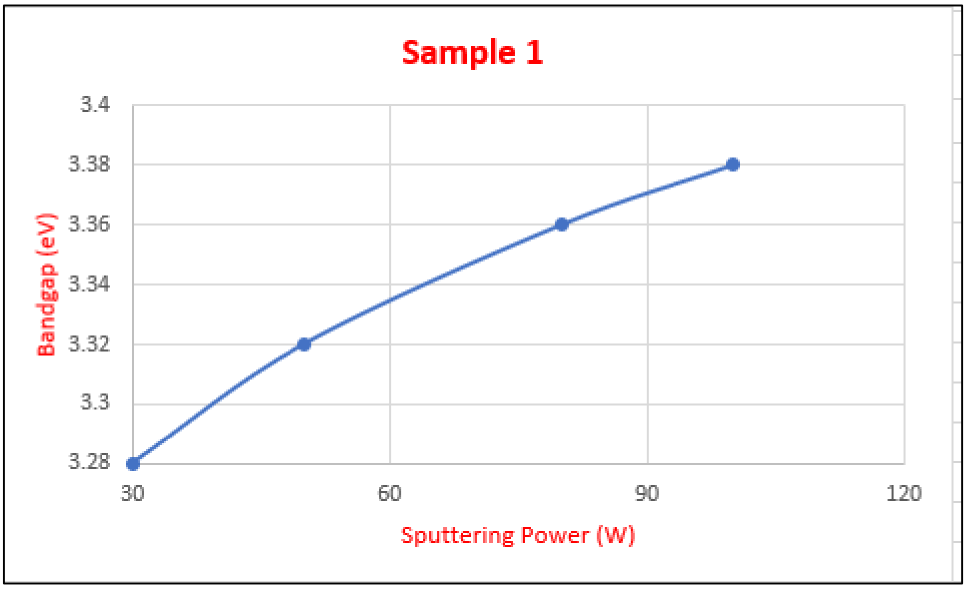

Figure 4.9 Optical band gap and Power of Sample 1

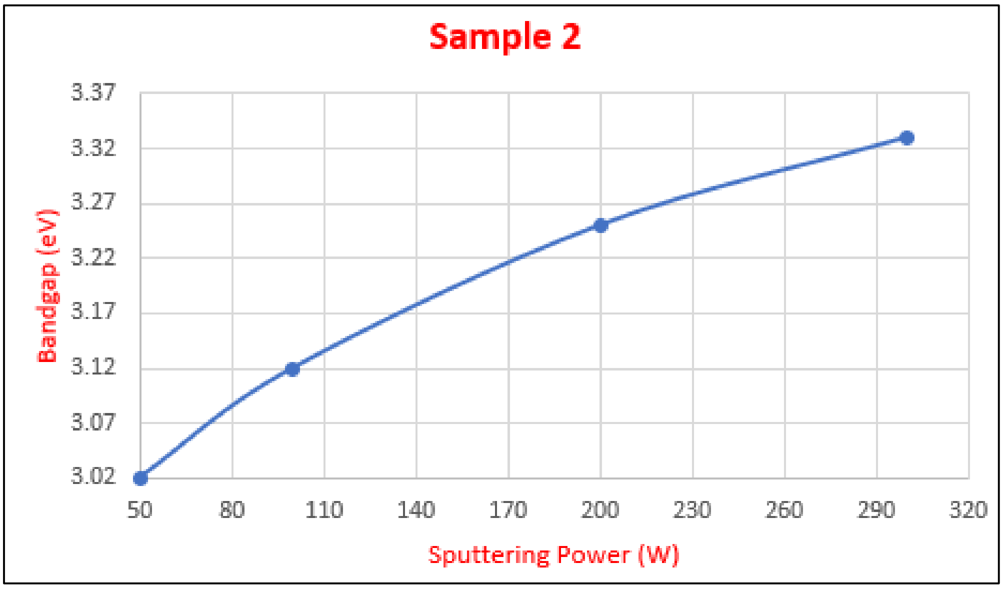

Figure 4.10 Optical band gap and Power of Sample 2

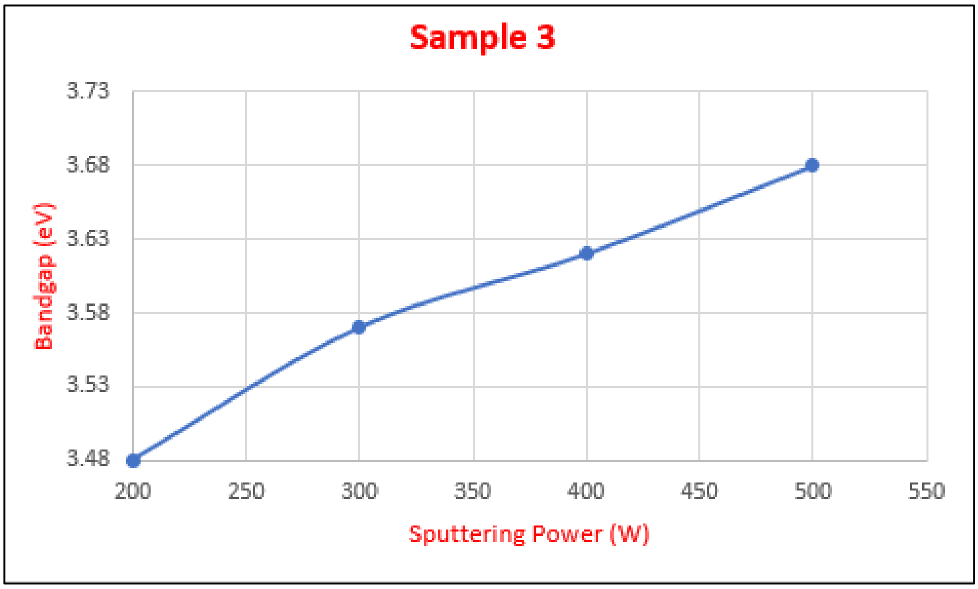

Figure 4.10 Optical band gap and Power of Sample 3

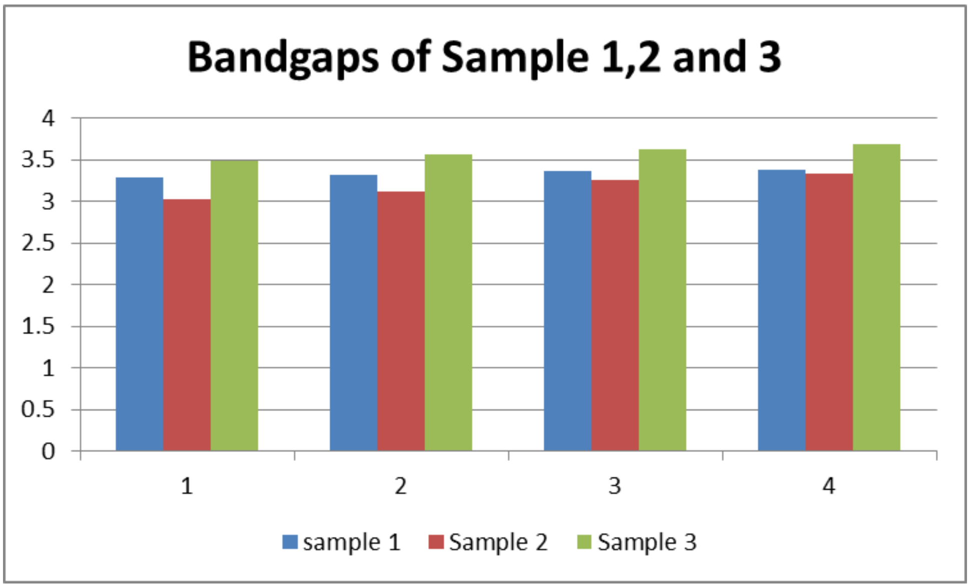

Figure 4.11 Combined band gaps from Sample 1, 2 and 3

From figure (4.8), (4.9) and (4.10), the trend shows that optical band gap of sample 1, 2 and 3 increases with increasing the sputtering power (W). As the higher energy, the wavelength will be shorter. Wide-band gap devices therefore are useful at shorter wavelengths.

Figure 4.11 shows the band gap trends of sample 1, 2 and 3. This is the bar diagram of sample 1 2 and 3 with the sputtering power (W) variation. This bar chart shows that the optical band gap of aluminium (Al) doped ZnO increase with the increase in power in the range of 30 to 500 W. This increase of optical band gap is due to the increase in optical transmittance characterized by UV Visible spectroscopy with the increase in RF sputtering power. The increase in sputtering power causes increase in the film thickness which leads to high optical transparency and results in the widening of band gap.

CONCLUSION

To summarize, the deposition of thin films on soda lime, borosilicate, and simple glass substrates using the AZO technique and radio frequency magnetron sputtering method was successful. The study aimed to investigate the effect of power (W) on the optical properties of the films. Films exhibited a hexagonal wurtzite structure, with a predominant growth orientation along the (0 0 2) plane and the c-axis perpendicular to the substrate. As the sputtering power increased, the crystallites in the AZO films decreased in size, and there was a gradual change in preferential orientation. The structural graphs in sample 1, 2 and 3 were plotted between Bragg's angle (2θ) and Intensity (a.u). Transmittance measurements were carried out to achieve the desired optical properties of AZO thin films. It was found that film thickness had a significant impact on the optical band gap, with the band gap of samples 1, 2, and 3 increasing with the sputtering power (W). As the energy increases, the wavelength becomes shorter, making wide-band gap devices more useful at shorter wavelengths compared to other semiconductor devices. The optical band gap of aluminium doped zinc oxide also increased with increasing sputtering power in the range of 30 to 500 W. The increase in sputtering power led to an increase in film thickness, resulting in higher optical transparency and a widening of the band gap.

LIMITATIONS

- Access to the articles and the journals relevant to this research topic available online was limited.
- Research material related to the synthesis and experimentation was limited.

RECOMMENDATIONS

- Synthesis of AZO via RF sputtering method leads to the increase in optical transparency and increase in the optical band gap of zinc oxide with respect to various sputtering powers.
- These highly transparent materials can served as potential oxides for transparent conducting oxides and displaying technologies.

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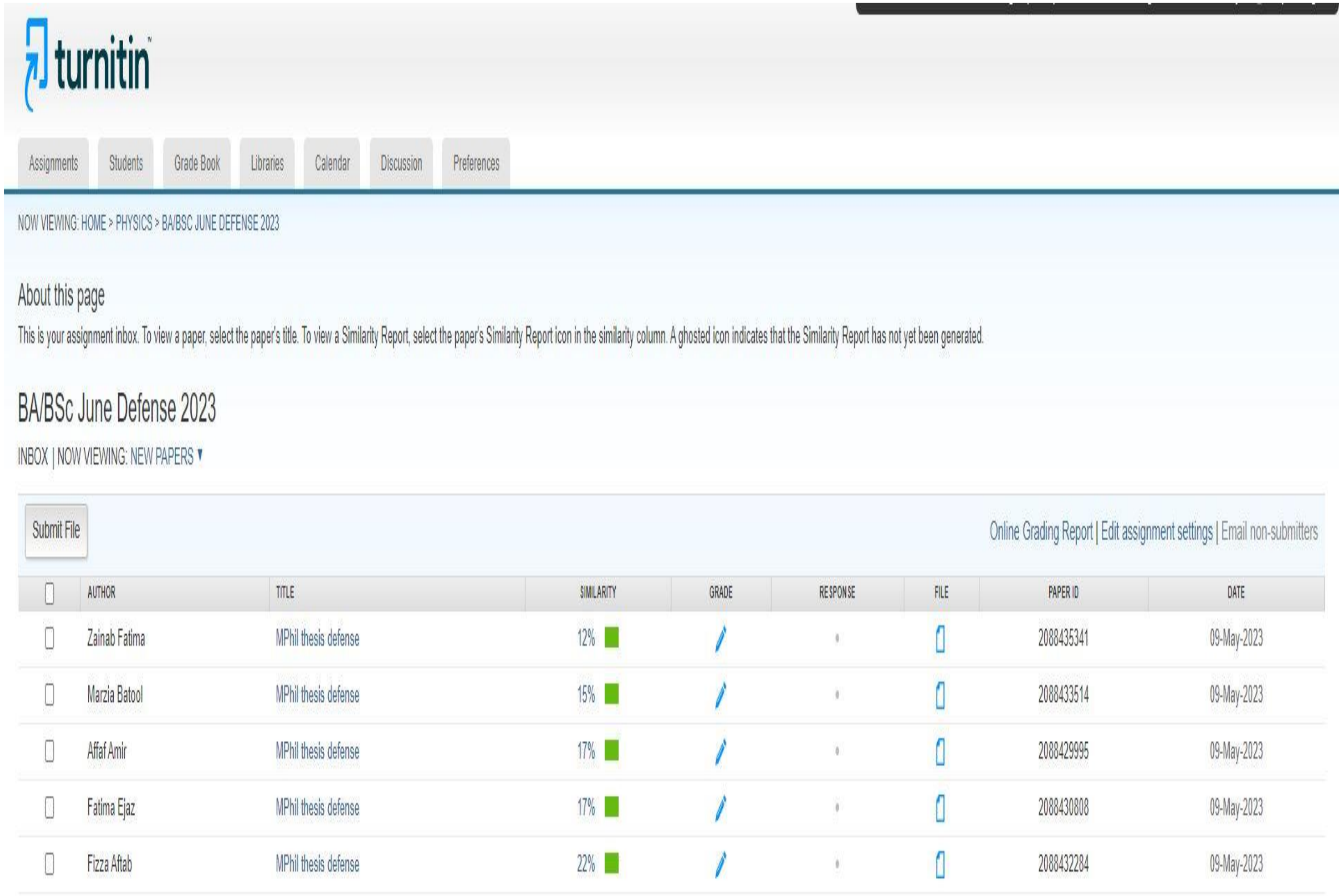

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