THE EFFECT OF DEPOSITION TEMPERATURE ON STRUCTURAL AND OPTICAL PROPERTIES OF CdS THIN FILM BY USING CHEMICALBATH DEPOSITION METHOD.

A thesis submitted to the department of physics in partial fulfillment of the requirement for the degree of Master of Science in solid state physics.

By

Dawit Ewnetie Temesgen

Hawassa, Ethiopia

May, 2024

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A thesis submitted to the department of Physics College of natural and computational science school of graduate.

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In partial fulfillment of the requirements for the degree of master science in physics (solid state physics)

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ABSTRACT

Cadmium sulphide is an intrinsic n-type semiconductor material with the chemical formula CdS. CdS thin films where deposited on glass substrates using cadmium sulphate as the cadmium ion source, thiourea as the sulphur source, and ammonia as the complexing agent through the chemical bath deposition method . The effect of deposition temperature ranging from 40^0C to 80^0C in 10^0C intervals on the structural and optical properties of thin films was investigated. The films were annealed at 300^0C for 1:30 hours. The CdS thin films were characterized using XRD for structure and UV-VIS spectrophotometer for optical property determination. Optical investigations revealed that CdS exhibited high absorption in the visible region, with the optical band gap from 1.80 eV to 1.37 eV as the temperature increased. This indicates an inverse relationship between deposition temperature and band gap energy, making these thin films suitable as absorber materials for solar cell fabrication. XRD analysis showed that the deposited CdS thin films had a simple hexagonal crystal structure with preferred orientation along the (002) plane. The intensity of the sharp peak indicates that the sample is highly crystalline. Additionally, the crystalline size of the CdS thin films increased with the higher bath temperatures.

Generally, varying the deposition temperature had effect on the structural and optical properties of cadmium sulphide thin films.

Key words: Thin films, CdS, Optical properties, Structural properties, Chemical bath deposition.

Table of Contents

LIST OF FIGURES

LIST OF TABLES

ABBREVIATIONS AND ACRONYMS

CdS	Cadmium sulphide
XRD	X-ray Diffraction
UV-VISS	Ultraviolet-Visible spectroscopy
CBD	Chemical bath deposition
CIGS	Copper indium gallium sulfide
CuInSe	Copper indium selenide
CuInGaSe	Copper indium gallium selenide
SEM	Scanning electron microscope
EDX	Energy dispersive X-ray spectroscopy
XPS	X-ray photoelectron spectroscopy
LEDs	light-emitting diodes
CdTe	Cadmium telluride
GaAS	Gallium arsenide
GaP	Gallium phosphorus
GaN	Gallium nitride
CdSe	Cadmium selenide
InSb	Indium antimony
InAs	Indium arsenide
InP	Indium phosphide
AlAs	Aluminum arsenide
PbS	Lead sulphide
PbSe	Lead selenide
ZnS	Zinc sulfide
ZnSe	Zinc selenide
Cu_2S	Copper sulfide
PbTe	Lead telluride
PEC	Photo-electrochemical
DSSCs	Dye sensitized solar cells
TEM	Transmission electro n microscopy
KSP	Solubility product

FWHM	Full Wave Half Maximum
JCPDS	Joint committee on powder diffraction standards
MOCVD	Metal organo chemical vapour deposition
SILAR	Successive ionic layer adsorption and reaction
CVD	Chemical vapour deposition
AFM	Atomic force microscopy
HgTe	Mercury telluride
Ge	Germanium
S	Sulfur
Te	Tellurium
P	Phosphorus
Se	Selenium
hν	Incident photon energy
IP	Ionic product
Eg	Band gap
nm	Nanometer
^{0}C	Degree centigrade
D	Grain size of the crystallite
KSP	Solubility product
eV	Electron volt
ν	Frequency incident beam
h	Planck's constant
λ	Wavelength
A	Absorbance
IR	Infrared ray
Å	Angstrom
θ	Scattering angle
d	Atomic spacing
Kv	Kilovolt
mA	milliampere

CHAPTER -ONE

1. GENERAL INTRODUCTION

Thin film is a material created by the random nucleation and growth processes of individually condensing / reacting atomic / ionic / molecular species on a substrate. The structural, chemical, metallurgical and physical properties of such materials are strongly dependent on a number of deposition parameters and thickness. Thin films encompass a considerable thickness range, varying from few nanometers to tens of micrometers and thus are best defined in terms of growth processes rather than thickness. The atomistic random nucleation and growth processes give new exotic properties to thin film materials .These properties can be controlled and reproduced by precisely modulating a range of deposition parameters .The thin film is a traditional well-established material technology. However, thin film technology is still being developed on a daily basis since it is a key in the twenty first century development of new materials such as nanometer materials and/or a man-made super lattices [1]. Thin film studies have directly or indirectly advanced many new areas of research in solid state physics and chemistry which are based on phenomena uniquely characteristic of the thickness, geometry and structure of the film. The phenomenal rise in thin film researches is no doubt due to their extensive applications in the diverse fields of electronics, optics, space science, aircrafts, defense and other industries. These investigations have led a numerous inventions in the forms of active devices and passive components, piezo-electric devices, micro-miniaturization of power supply, rectification and amplification, sensor elements, storage of solar energy and its conversion to other form, magnetic memories, super conduction films, interference filters, reflecting and antireflection coatings and many others. Thin film materials are the key elements of continued technological advances made in the fields of optoelectronic, photonic and magnetic devices. The processing of materials into thin films allows easy integration into various types of devices. The properties of material significantly differ when analyzed in the form of thin films. Most of the functional materials are rather applied in thin film form due to their specific electrical, magnetic, optical properties or wear resistance. Thin film technologies make use of the fact that the properties can particularly be controlled by the thickness parameter. Thin films are formed mostly by deposition, either physical or chemical methods.

Thin films, both crystalline and amorphous, have immense importance in the age of high technology. Few of them are: microelectronic devices, magnetic thin films in recording devices, magnetic sensors, gas sensor, A. R. coating, photoconductors, IR detectors, interference filters, solar cells, polarizer's, temperature controller in satellite, superconducting films, anticorrosive and decorative coatings [2]. Thin film deposition manufacturing processes are at the heart of today's semiconductor, solar panel, hard disk drive and optical device industries. Thin films can now be made in a variety of ways. The techniques can be divided into physical methods (top down approach) and chemical methods (bottom -up approach) [3]. Chemical bath deposition is a technique for depositing thin semiconductor films on substrates immersed in dilute solutions containing metal ions and hydroxide, sulfide, or selenide ion sources [4].

This thesis is primarily concerned with the effect of deposition temperature on structural and optical properties of CdS thin films by using chemical bath deposition method.

1.1 Semiconductor materials

Semiconductor materials are defined as materials in solid form whose conductivity has a value between conductors and insulators. Semiconductor materials play an important role in the advances in the modern electronics industry in the twenty-first century and in the industrial applications of many electronic devices. These materials include many materials such as silicon, gallium arsenide, germanium, cadmium sulfide, and cadmium telluride, which are widely used today. From the first silicon integrated circuits produced in semiconductor technology, high-tech microprocessors, solar cells, and many other electronic devices have developed rapidly to the present day [5]. The two general classifications of semiconductors are the elemental semiconductor materials, found in group IV of the periodic table, and the compound semiconductor materials, most of which are formed from special combinations of group III and group V elements.

1.1.1 Classification of Semiconductors

Semiconductors are also classified in two. Those are elemental and compound semiconductor.

1.1.1.1 Elemental semiconductors

The best-known semiconductor is of course the element Si. Together with germanium (Ge), it is the prototype of a large class of semiconductors with similar crystal structures. The crystal structure of Si and Ge is the same as that of diamond and α-tin (a zero-gap semiconductor also known as "gray" tin).

In this structure each atom is surrounded by four nearest neighbor atoms (each atom is said to be four-fold coordinated), forming a tetrahedron. These tetrahedrally bonded semiconductors form the mainstay of the electronics industry and the cornerstone of modern technology. Some elements from the groups V and VI of the periodical table, such as phosphorus (P), sulfur (S), selenium (Se) and tellurium (Te), are also semiconductors. The atoms in these crystals can be three-fold (P), two-fold (S, Se, Te) or four-fold coordinated. As a result, these elements can exist in several different crystal structures and they are also good glass-formers. For example, Se has been grown with monoclinic and trigonal crystal structures or as a glass (which can also be considered to be a polymer) [6].

1.1.1.2 Compound Semiconductors

A compound semiconductor is a semiconductor compound composed of elements of at least two different species. Compound Semiconductors offer high performance (optical characteristics, higher frequency, and higher power) than elemental semiconductors and greater device design flexibility due to mixing of materials. Examples are gallium arsenide (GaAs), indium arsenide (InAs), indium phosphide (InP), and gallium nitride (GaN). Compounds formed from elements of the groups III and V of the periodic table (such as GaAs) has properties similar to their group IV counterparts. In going from the group IV elements to the group III-V compounds, the bonding becomes partly ionic due to transfer of electronic charge from the group III atom to the group V atom. The iconicity causes significant changes in the semiconductor properties. It increases the coulomb interaction between the ions and also the energy of the fundamental gap in the electronic band structure. Iconicity becomes even larger and more important in the group II-VI compounds such as zinc sulphide (ZnS). As a result, most of the groups II-VI compound semiconductors have band gaps larger than 1eV. Exceptions are the compounds containing the heavy element mercury (Hg). Mercury telluride (HgTe) is actually a zero band gap semiconductor (or a semimetal) similar to gray tin. While the large band gap group II-VI compound semiconductors have potential applications for displays and lasers, the smaller band gap group II-VI semiconductors are important materials for the fabrication of infrared detectors [6]. Cadmium Sulphide (CdS) is one of the most important group II–VI based semiconductor with a direct band gap of 2.42eV at room temperature. CdS polycrystalline thin films is a representative material with many applications such as large area electronic devices and solar cells [7].

Table1: Common binary and ternary semiconductors [1].

Periodic table Group	Binary compounds	Ternary compounds
II-VI	CdS, CdSe, CdTe, ZnS, ZnSe, ZnTe	$Hg_{1-x}Cd_xTe$, $Cd_{1-x}Zn_xTe$, $ZnS_{1-x}Se_x$, $Cd_{1-x}Zn_xS$, $Cd_{1-x}Zn_xSe$
III-V	GaP, GaAs, GaSb, InP, InAs, InSb	
IV-VI	PbS, PbSe, PbTe	$Pb_{l-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$, $PbS_{1-x}Se_x$
IV-IV	SiC, $Si_{1-x}Ge_x$	
V-VI	Bi_2Te_3	
I-III-VI_2 or II-VI-V_2 Chalcopyrite	$AgGaS_2$, $AgGaSe_2$	$CuInS_2$, $CuInSe_2$

1.1.2 Semiconductor thin films

Properties of semiconductor thin films are directly related to the production technique, and their thickness ranges from a few nanometer s to hundreds of micrometers. In general, semiconductor thin films are produced in one or more thin layers. Common applications of such structures include many electronic materials such as transistors, sensors, and photovoltaic devices. Especially in recent years, semiconductor thin films can be obtained compared to the use of bulk materials, making it a promising ideal candidate in the electronic material industry due to its wide variety of properties. First of all, a wide range of chemical, electrochemical, and physical deposition techniques enables the low-cost production of semiconductor material on large areas of the desired geometry and structure. In addition, single or multi-crystalline structures with complex geometry and even microstructures of nano crystalline thin films can be easily obtained by changing the method, temperature, substrate, and other production parameters depending on the method. Industrial applications of electronic materials come to life with different junction types between different semiconductor materials to improve the electrical properties of thin films. Semiconductors thin film form an essential part of many modern electronic applications, such as mobile phones, LED displays, and photovoltaic cells [5].

1.2 General Property of Cadmium Sulphide

Cadmium sulphide (CdS) is among the binary compounds of group II-VI family and its thin films are widely used in various materials such as light emitting diodes (LEDs), solar cells, electronic and optoelectronic devices [8]. Group II-VI semiconductors such as cadmium sulfide (CdS),zinc sulfide (ZnS), cadmium selenide (CdSe), and ZnSe are used as buffer layers in Cu (In, Ga) (S, Se) (CIGS) photovoltaic devices. Cadmium sulfide (CdS) is the most commonly used buffer layer. Cadmium sulfide (CdS) is an n-type semiconductor with a band gap of 2.42 eV at room temperature. Thus CdS thin films have been used widely as window layers in solar cells with an absorber layer of cadmium telluride (CdTe), copper sulfide (Cu_2S), or copper indium selenide (CuInSe) [9]. Cadmium sulfide has, like zinc sulfide, two crystal forms , the more stable hexagonal wurtzite structure (found in the mineral Greenockite) and the cubic zinc blende structure (found in the mineral Hawleyite).

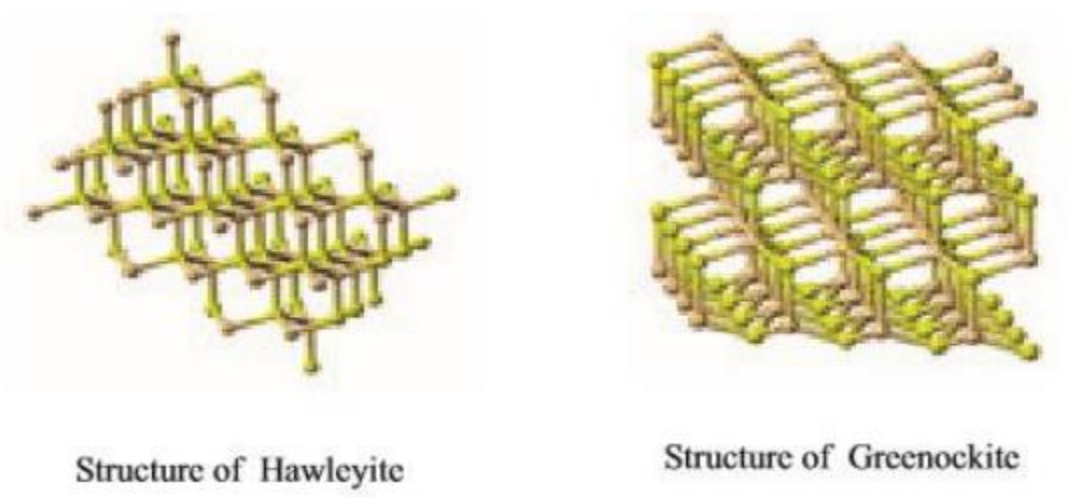


Figure1: Structure of cadmium sulfide [10].

Additionally, CdS exhibits photoconductivity, where its electrical conductivity increases upon exposure to light. However, cadmium sulphide is toxic and poses environmental risks due to release of cadmium ions. Proper handling and disposal are crucial when working with CdS to prevent harm to human health and the environment.

1.3 Statement of the problem

Cadmium sulphide (CdS), a wide energy gap semiconductor has emerged as an important material due to its applications in photovoltaic cell as window layers, optical filters and multilayer light emitting diodes, photo detectors, thin film field effect transistors, gas sensors and transparent conducting semiconductor for optoelectronic devices [11].

In this research, a chemical bath deposition (CBD) technique was employed to synthesize CdS thin films. The process utilized optimized proportion of $CdSO_4$ as a cadmium ion source, thiourea as the sulphur source and ammonia as complexing agents. The resulting cadmium sulphide thin films were characterized for their structural and optical properties using XRD and UV-VIS spectrophotometer. While previous studies have explored the effect of solution PH and deposition time on CdS thin film growth, there is gap in the research regarding the influence of deposition temperature on CdS thin film properties. Annealing at 300^0C for 1 hour and 30 minutes is different from previous studies because it specifically focuses on the impacts of deposition temperature and a specific annealing condition, which has not been extensively explored before in relation to CdS thin film growth. By systematically varying the deposition temperature and studying the resulting thin film characteristics such as crystallinity and optical properties, we can determine how deposition temperature influences CdS thin film properties. This comprehensive study will help in understanding the impact of deposition temperature on CdS thin film growth and properties.

1.4 Research Objectives

1.4.1General objective

- The general objective of this work is to investigate the effect of deposition temperature on structural and optical properties of cadmium sulphide (CdS) thin film by using chemical bath deposition method.

1.4.2 Specific objectives

The specific objectives of this work are:

- To synthesize CdS thin film on glass substrates using chemical bath deposition at different temperatures ranging from 40^0C to 80^0C with 10°C increments.
- To analyze the structural changes in CdS thin films at different deposition temperatures, focusing on the variation in grain size.

- To determine the relationship between deposition temperature and the optical properties of CdS thin films, specifically focusing on changes in band gap energy.

1.5 Significance of the study

This study will provide valuable insights for variety of industries and scientific fields due to the unique properties and versatile applications of CdS. As semiconductor material, cadmium sulphide is utilized in electronic devices like solar cells, light sensors, and photoresistrors for its ability to conduct electricity under specific conditions; its bright and stable yellow color also makes it a popular pigment in paints and coatings. Specifically, this research will contribute to a better understanding of how deposition temperature influences the band gap energy of CdS thin films, which directly impacts the efficiency of CdS-based solar cells and other optoelectronic devices.

1.6 Thesis structure

The thesis is structured into five chapters. The first chapter provides general introduction, including a definition and classification of semiconductors. It then delves into general properties of cadmium sulphide (CdS).The chapter concludes with a Statement of the problem, the objectives of the present work, and a description of the thesis is organization. The second chapter introduces thin film materials and concludes with an extensive review of CdS thin films deposited using the chemical bath deposition method. Chapter three discusses Chemical bath deposition, thin film deposition techniques, characterization techniques, and experimental details. Chapter four presents the results and analysis of the thin film, followed by a discussion. Finally, chapter five offers conclusions and future study based on the findings of the research.

CHAPTER- TWO

2. LITERATURE REVIEW

In this chapter, the general aspects of thin film materials, and review of synthesis and characterization of CdS thin films prepared by chemical bath technique are presented in some detail.

2.1 Thin films

Thin film is a small-dimensional material on the substrate produced by intensifying, one-by-one, and ionic/molecular/atomic species of matter. The thickness of thin film is generally less than a number of microns. In fact, there is another type of film that is called thick film, which is known as a small-dimensional material formed by accumulating great grains/aggregates/clusters of ionic/molecular/atomic species or thinning a three-dimensional material. Factually, over the past 50 years, the thin films have been used for manufacturing optical coatings, electronic devices, decorative parts, and instrument hard coatings. The thin film is a conventional well-established material technology. In contrast, since the thin film technology is a main improvement of novel materials such as nanometer materials in the twenty-first century, it is still being developed on a daily basis [12].

2.2 Literature review on CdS thin film by CBD method

In this section, some works done by different scholars to synthesize CdS thin films using CBD have been reviewed.

Castillo et al.(2011), deposited the CdS thin films on glass slide substrates using the chemical bath deposition (CBD) method with 0.1M cadmium nitrate tetra hydrated ($Cd(NO_3)_2 \cdot 4H_20$), 1M thiourea [$(NH_2)_2CS$], pH 11 buffer, at 80 °C and 0.5 M glycine (NH_2CH_2COOH) employed as an alternative complexing agent for the synthesis of CdS thin films. The product was characterized with X- ray diffraction, atomic force microscope, optical absorption and X-ray photoelectron spectroscopy (XPS). XRD pattern show that atypical CdS thin film obtained by using glycine as complexing agent in the CBD process. This pattern displays an intense peak at about 26.7° and weaker diffraction signals at about 28.6, 48.3 and 52.3°, which can be assigned to the reflections by (002), (101), (103) and (112) planes of the CdS hexagonal crystalline phase.

The optical properties of CdS thin films, measured using UV/Vis/NIR spectrometer. The film presents a low absorbance in the region from 450 to 900nm, i.e. high transmission. XPS chemical analysis was practiced without deep profile, just in order to estimate the very superficial al chemical composition of the CdS thin films, as can be observed in a roughly way from the XPS pattern, the identified binding energies peaks show the main presence of Cadmium and Sulphur, but some additional peaks are also present. The high purity of the sample was corroborated by the XPS measurements [13].

In 2009 Moualkia, Hariech and Aida, Chemical bath deposition was used to prepare and the study of the structural and optical properties of CdS thin films. NH_4OH, $CdSO_4$, and CS $(NH_2)_2$ are used in a reaction. The films properties were researched in relation to bath temperature and deposition time. Transmittance is fine at various baths a temperature range of 55°C to 65°C. As the temperature of the solution rises, the size of crystallites in CdS thin films decreases. The structural investigation was carried out using X-ray diffraction analysis properties of the obtained films. Crystallite size and other structural parameters have been assessed. The transmission spectra the films acquired have been reported in the UV visible range, indicating that they have a relatively high transmission coefficient (70%). The deposition circumstances have a strong influence on the optical band gap according to the transmittance data analysis, with a gap in the straight band varying Deduced from 2.0 eV to 2.34 eV. The dark conductivities the deposition rate of CdS films can be controlled by either the deposition rate or the deposition rate of CdS films time or the bath temperature, according to the electrical characterization. Deposition when the temperature is low (50°C) and for a long time times have high optoelectronic capabilities, meaning that these circumstances are excellent for manufacturing CdS thin films for optoelectronic CIS solar cells, for example, have a buffer layer [14].

Lahewil et al. (2012) reported CdS nanostructure deposited on glass substrates at different thiourea concentrations Cd: S 0.05:0.01, 0.03, 0.05 and 0.1mol/l. All films show a strong preferential orientation at 2θ =26.60 of either H (002) or C (111) planes. The CdS nanostructure deposited on glass substrate at 0.1mol/l, shows three narrow peaks corresponds to (100), (002) and (101) planes, respectively [15].

Lee and Tsakalakos (1997) studied CdS thin films consisting of the quantum dots grown by solution growth technique on slide glass substrates, and the influences of growth conditions such as ammonia concentration, growth temperature, and growth time on the structural and optical properties of CdS thin films. From XRD measurement results, CdS thin films at every deposition condition were found to have hexagonal structure. Depending on the various growth conditions, the film thickness ranged from 37 nm to 220 nm and the grain size ranged from 7.4 nm to 26.5 nm. For low ammonia concentration, the increase of grain size and film thickness was observed with increasing growth temperature. This led to the abrupt reduction of band gap which was ascribed to the large increase of film thickness and grain size in this case. For low growth temperature, the band gap decreased substantially with an increase in ammonia concentration. The energy band gap (Eg) was calculated from absorption coefficients obtained from the optical transmittance, and Eg varied from 2.42 eV to 2.6eV, depending on the growth conditions [16].

Tizazu et al. (2017), Deposited well adherent Nano crystalline cadmium sulphide thin films on silica glass substrates from acidic chemical baths by employing tartaric acid and hydrazine as complexing agents for the first time. The pH of the bath was about 2.35 and the depositions were carried out at bath temperatures of 60 °C and 70 °C. The films were characterized by a variety of techniques. Powder X- ray diffraction patterns of the films exhibited a well crystallized hexagonal structure with a preferred orientation along the (002) plane. Scanning electron microscope investigation showed that the films are formed from spherically shaped grains. The EDAX result revealed that the deposited films had very good stoichiometry. The band gap of the thin films obtained by optical absorption spectroscopy, were 4.12 eV for the films deposited at 60 °C and 3.89 eV for films deposited at 70 °C [17].

In 2007 Lee structural and optical properties were investigated characteristics of chemically produced Films made of CdS as a function of substrate. The substrates (they employed the same materials) impact the structural phase of CBD CdS thin films). Different substrates yielded hexagonal or cubic phases; although hexagonal was obtained on a glass substrate is consistent with the help of findings. According to certain studies, Low ammonia concentration in solution, since Cd $(OH)_2$ is clearly visible suspension leads to the manufacture in the wurtzite process of CdS. The edge of optical transmission was smoother the films were annealed at 200°C and 300°C, respectively. Suggesting the temperature at which the annealing takes place promotes crystalline nature.

They additionally observed that each and every film had good visible transmission of light, implying that CdS thin films produced under comparable circumstances by CBD might be employed the energy band gap in solar cells as a window material is 2.42 eV [14].

Thirumavalavan et al. (2015) reported CdS thin films by CBD method. The CdS films were characterized for structural, morphological, optical, & electrical properties. SEM studies are examine to identify uniform grains with uneven spherical shaped, distributed over the entire surface of the substrates. AFM analyses were employed over the film to confirm uniform deposition of film over the entire substrate surface. EDAX analysis confirms the stoichiometric deposition of film. Optical studies of the deposited film confirmed an optical energy gaps ranging from 1.74 to 1.87 eV depending on the substrate temperature. The optical band gap of CdS thin film was estimated by UV-vis spectroscopy. X-ray diffraction (XRD) studies are used to identify the polycrystalline in nature with the hexagonal crystal structure [18].

The researchers report above shows that the effect of deposition temperature on cadmium sulphide thin film deposited by CBD is very few. This study aims to fill this gap and add knowledge on the effect of deposition temperature on CdS thin film properties by annealing at 300^0C for 1 hour and 30 minutes.

CHAPTER- THREE

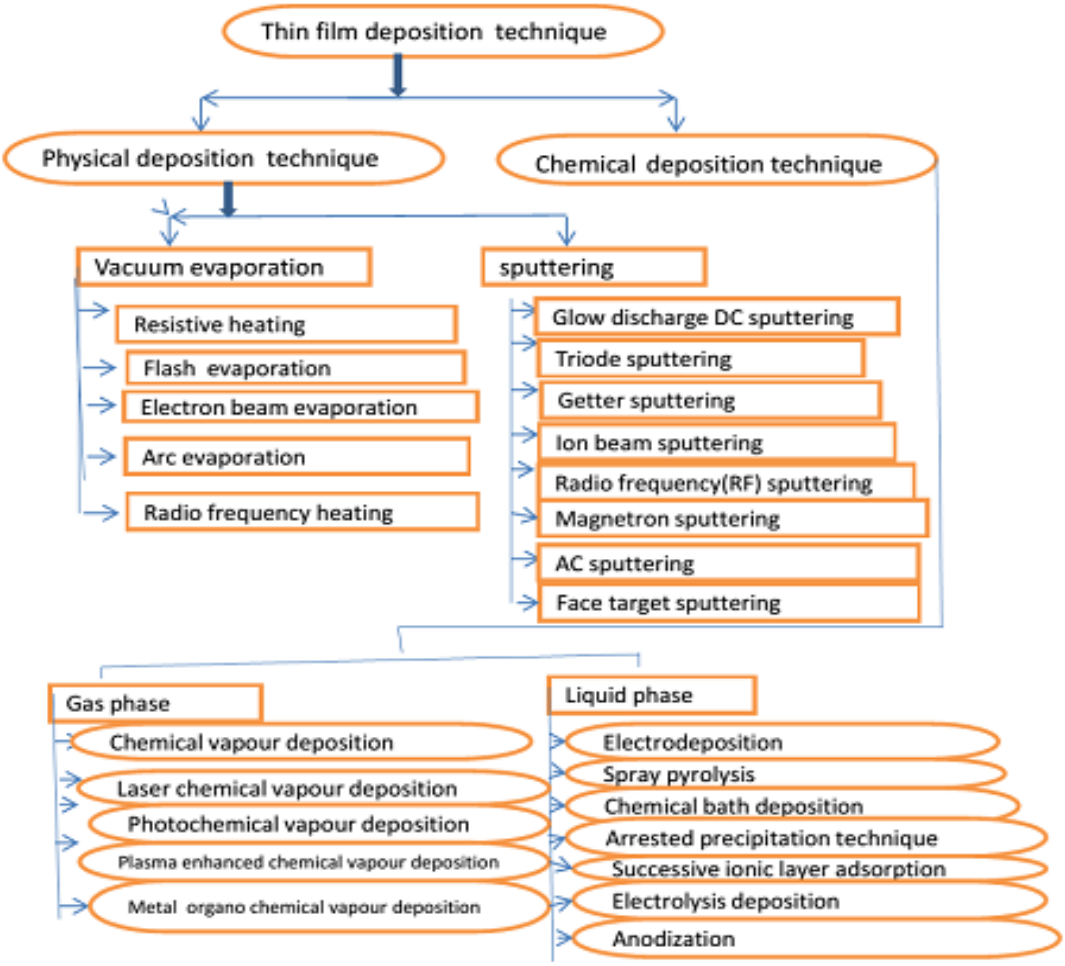
3. METHODOLGY

3.1 Thin film deposition techniques

Thin films play an important role in the present day technology development and techniques of film deposition offer a major key to the fabrication of solid-state microelectronic devices. Thin film deposition is the process of placing the layers of thin film on another surface, usually a crystalline surface. The vast varieties of thin film materials, which consist of deposition process and fabrication techniques, spectroscopic characterization and optical characterization probes, were used to produce good devices [19]. Thin films can be fabricated in various ways. The techniques can be divided into physical methods and chemical methods.

- A physical method, the film material is moved from a target source with some form of energy to the substrate. This method is widely used in compound thin films. Under physical methods we have vacuum evaporation and sputtering, where the deposition has been transferred to gaseous state either by evaporation or an impact process.
- Chemical film fabrication method involves chemical reaction and the precursors are mostly components undergoing reaction at the substrate surface or in the vicinity of the substrate. Under chemical methods we have the gas phase chemical processes such as conventional chemical vapour deposition (CVD), laser CVD, metal organ chemical deposition (MOCVD) and plasma enhanced chemical vapour deposition. Liquid phase chemical techniques include electrodeposition, chemical bath deposition, electroless deposition, anodization, successive ionic layer adsorption and reaction (SILAR), spray pyrolysis etc. [1].

Table 2: Classification of thin film deposition techniques [1].



Any thin-film deposition technique involves three main steps:

1. Production of the appropriate atomic, molecular, or ionic species.

2. Transport of these species to the substrate through a medium.

3. Condensation on the substrate, either directly or via a chemical and/or electrochemical reaction, to form a solid deposit [20]. In principle, CBD can be used to deposit any compound that satisfies the following four basic requirements [21]:

- It should be possible to create the compound by simple precipitation. This generally, although not exclusively, refers to the formation of a stoichiometric compound formed by ionic reaction.
- The compound should be relatively (and preferably highly) insoluble in the solution used.
- The compound should be chemically stable in the solution.
- If the reaction proceeds via the free anion, then this anion should be slowly generated (to prevent sudden precipitation). If the reaction is of the complex decomposition type, then decomposition of the metal complex should similarly occur slowly.

  Of course there are other specific factors that need to be taken into account, particularly whether the compound will form an adherent film on the substrate or not. However, the preceding four factors are general requirements.

3.2 Chemical bath deposition

Chemical bath deposition (CBD is one of the solution phase methods useful for the preparation of compound semiconductors from aqueous solutions. It is widely used for the deposition of various metal chalcogenide thin films. It produces good deposits on suitable substrates by the controlled precipitation of the compounds from the solution. The method offers many advantages over other well-known vapor phase synthetic routes. It may allow us to easily control the growth factors such as film thickness, deposition rate and quality of crystallites by varying the solution pH, temperature and bath concentration. It does not require high voltage equipment, works at room temperature, and hence it is inexpensive. The only requirement for this deposition route is an aqueous solution consisting of a few common chemicals and a substrate for the film to be deposited [22]. Chemical bath deposition technique offers a means of intensively producing large are area sample, utilizing a technology readily adaptable to industrial production. The properties of the deposited material can be varied and controlled by proper optimization of the chemical baths and deposition conditions [23]. In these methods, substrates are stationary and solution is stirred with the help of magnetic stirrer. Water or paraffin baths with constant stirring are used to heat the chemical bath to the desired temperature. In some cases, stirring is continuous from room temperature, while in some cases, it is started after attaining the desired temperature [24].

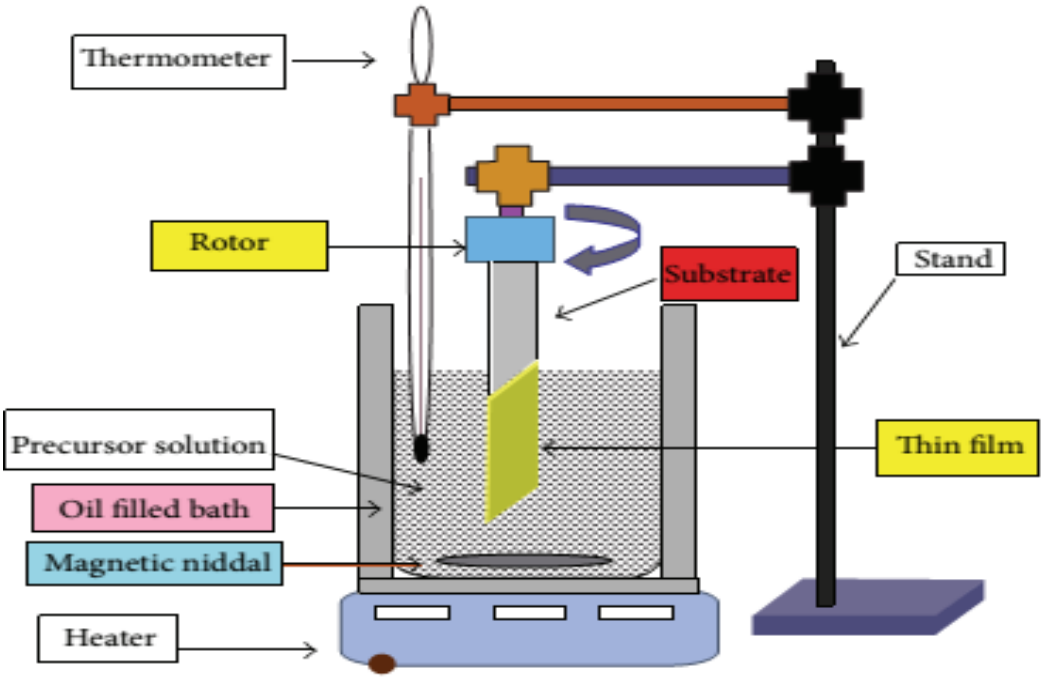


Figure 2: Experimental set up of CBD [25].

Many studies have been conducted,for about three decades, on chemical bath deposition (CBD) method for the preparation of thin films. Due to excellent productivity of this technique on a large scale and simplicity of the apparatus, it offered the most attractive way for the formation of thin films of oxides,semiconductors, chalcogenides and super-conducting oxides. The choice of this method arises from its low cost, ease of handling, possibility of application on a large surface, and simplicity of instruments for deposition [23].

Overall, while CBD techniques are versatile and cost- effective, they have several drawbacks that limit their applicability for applications. These drawbacks include limited material choices, non-uniformity, adhesion issues, substrate selectivity, environmental concerns, and poor control over thin film properties.

3.2.1 Basics of chemical bath deposition

The basic working principle behind the CBD process is similar to those for all precipitation reactions and it is based on relative solubility of the product. At a given temperature when the ionic product (IP) of reactants exceeds the solubility product (KSP), precipitation occurs. Whereas if the ionic product is less than the solubility product, then the solid phase produced will dissolve back to the solution resulting in no net precipitation [1].

Consider a saturated solution of sparingly soluble salt AB containing A^+ and B^- ions in contact with undissolved solid AB. In such situation an equilibrium is established between the solid phase AB and the ions (A^+ and B^-) which can be written as

$$AB\ (S) \Leftrightarrow A^+ + B^- \quad \ldots\ldots (3.1)$$

Applying law of mass action,

$$K = \frac{[A+]\,[B-]}{[AB]} \quad \ldots\ldots (3.2)$$

Where $[A^+]$, $[B^-]$ and [AB] are concentrations of A^+, B^- and AB in the solution, respectively. The concentration of pure solid is a constant number i.e.

$$[AB] = \text{a constant} = k' \ldots\ldots (3.3)$$

$$K = \frac{[A+]\,[B-]}{K'} \ldots\ldots (3.4)$$

Or

$$kk' = [A^+]\,[B^-] \quad \ldots\ldots (3.5)$$

Since K is equilibrium constant and k' is another constants, the products of kk' is also constant, say Ks, therefore Eq. (3.5) becomes

$$Ks = [A^+]\,[B^-] \quad \ldots\ldots (3.6)$$

The constant Ks is called solubility product (SP) and ($[A^+]$ $[B^-]$) is called ionic product (IP). When the solution is saturated the ionic product is equal to the solubility product. When the ionic product exceeds the solubility product i.e. IP/SP=S>1, the solution is supersaturated (S =degree of super saturation). Ions combine on the substrate and in the solution to form nuclei. Nucleation and growth of a material via CBD is determined by super saturation, this occurs when a solution containing a higher concentration of solute than the allowed solubility. If the ionic product is less than the solubility product, then the solid phase produced will dissolve back to the solution resulting in no net precipitation. This forms the basic principle behind any chemical deposition process [26].

3.2.2 Thin Film deposition mechanism in chemical bath deposition

There are four main mechanisms leading to compound formation, whose operation depends on the specific process and reaction parameters. The thin film growth in CBD occurs via the following four possible mechanisms.

1. Simple Ion-by-Ion Mechanism
2. Simple Cluster (Hydroxide) Mechanism

3. Complex-Decomposition Ion-by-Ion Mechanism

4. Complex-Decomposition Cluster Mechanism

3.2.2.1. Simple Ion-by-Ion Mechanism

In most of the CBD's, the ion-by-ion conceptually simplest mechanism, often assumed to be the operative one in general. It occurs by sequential ionic reactions. The general reaction for the mechanism.

$M^{n+} + X^{m-} \rightarrow M_m X_n$ (Adsorbed on the substrate) …….. (3.7)

The formation of solid $M_m X_n$ is based on the principle that when the ion product, $[M^{n+}][X^{m-}]$, exceeds the solubility product, Ksp , of $M_m X_n$, then $M_m X_n$ can form as a solid phase, although a larger ionic product may be required if super saturation occurs. If the ion product does not exceed Ksp, no solid phase will form, except possibly transiently due to local fluctuations in the solution, and the small solid nuclei will redissolve before growing to a stable size. For that reason, the precipitation process is an equilibrium rather than as a one-way reaction.

3.2.2.2. Simple Cluster (Hydroxide) Mechanism

In most of the CBD's, the preparative conditions are chosen so that the formation of metal hydroxide should be avoided. However, in reality, CBD's are quite often carried out under conditions where a metal hydroxide (or hydrated oxide) is formed. This might seem to imply that a precipitate of metal hydroxide $[M(OH)_n]$ is formed at the start of the CBD. In fact, the metal hydroxide formed is either as a colloid (rather than a precipitate) or as an adsorbed species on the substrate but not in the bulk of the solution. In this case metal chalcogenide ($M_m X_n$) is formed by reaction of X^{m-} ion with the $M(OH)_n$.

$$M^{n+} + OH^- \rightarrow M(OH)_n \quad \text{…… (3.8)}$$

Followed by

$$M(OH)_n + X^{m-} \rightarrow M_m X_n + nOH^- \quad \text{…….. (3.9)}$$

The deposition of the thin film takes place through the condensation of the metal and sulphide/selenide ions on this initial layer which acts as a catalytic surface.

3.2.2.3. Complex-decomposition ion-by-ion mechanism

In this mechanism, complexation of free metal cations (M^{n+}) by chalcogenide source (thiourea, thioacetamide) gives M-chalcogenide source complex ion. This is illustrated by the example of CdS deposition from thiourea.

$$Cd^{2+} (NH_2)_2CS = [(NH_2)_2CS - Cd]^{2+} \quad \text{…… (3.10)}$$

This ion is hydrolyzed by breaking the S-C bond to form CdS.

$[N H_2)_2CS - Cd]^{2+} + 2OH^- \rightarrow CdS + C N_2 H_2 + 2H_2O$……. …… (3.11)

This would lead to CdS formation in solution. If Cd^{2+} is adsorbed on the substrate (either directly or indirectly through a hydroxide linkage) then above reaction occurs and CdS is formed on substrate, the result would be film growth by ion-by-ion. This mechanism is also useful in acidic solution; thioacetamide decomposition at intermediate pH values, particularly in weakly acidic solution ($pH \geq 2$) has been suggested to occur through a thioacetamide complex.

3.2.2.4. Complex-Decomposition Cluster Mechanism

The complex-decomposition cluster mechanism is based on the formation of solid phase, instead of reacting directly with a free anion; it forms an intermediate complex with the anion-forming reagent. For CdS deposited from a thiourea bath the process can be described as:

$Cd (OH)_2 + (N H_2)_2CS \rightarrow Cd (OH)_2.SC (N H_2)_2$ …… (3.12)

$Cd (OH)_2$ is one molecule in the solid phase cluster. This complex or a similar one if contains ammine ligands then decomposes to CdS.

$Cd (OH)_2.SC (N H_2)_2 \rightarrow CdS + C N_2 H_2 + 2H_2O$ …… (3.13)

The S-C bond of the thiourea breaks, leaving the S bond to Cd. It is suggested that $Cd (OH)_2$ forms initially on the substrate and catalyzes the thiourea decomposition. The catalytic effect of the solid surface could be to decompose thiourea to sulphide ion and not necessarily to catalyze the complex-decomposition mechanism [25].

3.2.3 Factor influencing the deposition process

Deposition process: Generally, chemical bath deposition method is used to prepare thin films from cations with sulphide, selenide and telluride ions. The properties of films can be controlled by different deposition conditions such as pH, bath temperature, deposition time, complexing agent and nature of Substrate.

3.2.3.1 The influence of deposition time

Deposition time is one of the parameter which affects thin film deposition in CBD method. In most cases it has great influence on structural, morphological and optical properties of thin films. The growth of good quality semiconductor thin films proceeds to slow rate. This technique of CBD is ideally suited for producing uniform films with thickness in the (0.05 -0.3) μm range in most cases [27].

3.2.3.2 The influence of bath Temperature

The rise in bath temperature enhances the rate of diffusion and increases ionic mobility, hence the increase in conductivity of the bath. The increase in temperature increases the rate of crystalline growth favoring the course deposits. This increase in crystal size corresponds to decrease in polarization. At higher temperature, current densities increase, which increases the rate of nucleation, hence fine-grained, smooth deposits can be obtained [28].

3.2.3.3 Nature of Substrates

This factor plays an important role in the reaction mechanism and the adhesion of the deposited film. Hence, cleaning the substrate surface forms the first important step in the thin film deposition procedure. It may be non-crystalline solids e.g., glass of vitreous silica or crystalline such as cleavage plates of rock salt or mica. To select a particular substrate one has to take into consideration of the lattice parameter of the substrate so that it matches with the lattice parameter of the grown film, otherwise structural mismatch may create mechanical fracture in the film. It is also necessary to consider the melting point of the substrate material. It should be comparable with that of the film materials [29].

3.2.3.4 Effect of Concentration of Cation and Anion Sources

Chemical bath composition is critical for synthesis of good quality of thin films. The nature of the reactants influences the whole physical and chemical properties of the deposited thin film. By changing the composition of the reactive solution, competition between the processes of homogeneous and heterogeneous nucleation could be altered to favor thin film growth. Nature of the reactants influences the composition of the products [30].

3.3 Thin film characterization techniques

In the advancement of science and technology the discovery of novel materials those are having varied characteristics and applications have played an important role.

The complete characterization of any material consists of phase analysis, compositional characterization, structural elucidation, microstructural analysis and surface characterization, which have strong bearing on the properties of materials. In this study Cadmium Sulphide (CdS) thin films were deposited on glass substrate using chemical bath deposition method.

The structure and optical properties of the CdS thin films were studied by using X-ray diffraction (XRD) and UV-Visible spectrophotometer respectively.

3.3.1 X-ray diffraction (XRD)

X-ray diffraction (XRD) is a simple and non-destructive analysis technique which provides means to identify different phases and their distribution in the sample, texture, evaluate average grain size, internal stress, etc. X-rays are electromagnetic waves with wavelength (0.5-50 Å) comparable to atomic separation distances. When propagating through a crystal, the X-rays interact with the lattice and are diffracted according to the Bragg's law

$$2d\sin\theta = n\lambda \quad \text{...} \quad (3.14)$$

Where d is the atomic spacing, θ is the scattering angle, n is an integer number, and λ is the wavelength.

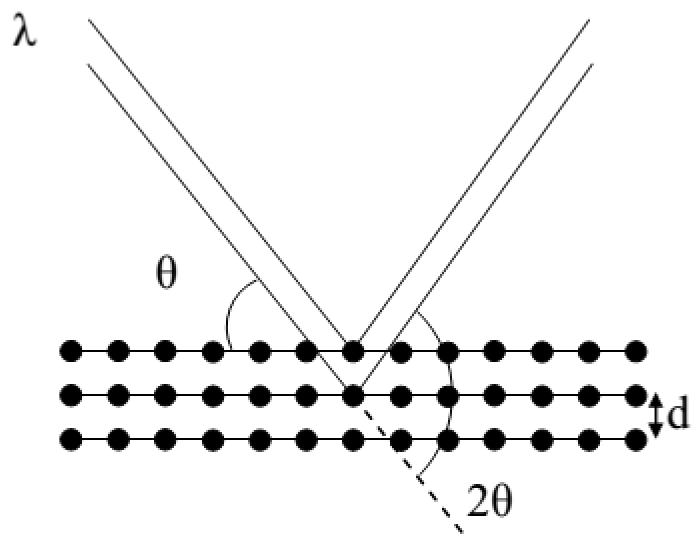


Figure 3: Schematic illustration of an XRD θ/2θmeasurement.

As the combination of constituent atoms, crystal structure, and lattice constants is different for different materials/phases, XRD results in a unique set of diffraction angles and diffracted beam intensities, which make phase identification possible [31].

The grain size of the crystallite is obtained by substituting values of Full Width at Half Maximum (FWHM) in the well-known Debye Scherrer formula.

$$D = \frac{0.9\lambda}{\beta\cos\theta} \quad \text{...} \quad (3.15)$$

Where D is grain size of the crystallite, K = 0.94, (λ=1.54059 Å) is the wavelength of the X-ray source used, β is the broadening of the diffraction line measured at half of its maximum intensity in radians (FWHM) and θ is the angle of diffraction at the peak [32].

3.3.2 Ultraviolet-Visible Spectroscopy (UV-VISS)

UV-Vis spectrometers collect the data over the required range and generate the spectrum of the compound under analysis as a graph representing the transmittance (or the absorbance) as a function of wavelength along the abscissa, given in nanometers, the recommended unit in this region. This region of the spectrum is conventionally divided into three sub -domains termed near UV (185–400 nm), visible (400–700 nm) and very near infrared (700 – 1100 nm). One of the defining features of a semiconductor is the band gap, which separates the conduction and valence bands. Upon absorption of light, an electron is promoted from the valence to the conduction band. The wavelength of light absorbed and emitted from this material is determined by the width of the band gap. The UV-VIS absorption spectroscopy is frequently used to characterize semiconductors thin films and to determine the band gap of then nanostructure materials and also to understand the quantum confinement of the nano particles[1].

3.4 Chemicals and experimental procedures

3.4.1 Materials Used

Apparatus such as beaker, volumetric flask, substrate holder, and water bath, measuring cylinder, stirring rod, magnetic stirrer, glass substrate or glass slide were first washed with detergent and rinsed with distilled water and dried in open air. Other materials, like thermometer, beam balance and heater were also used.

3.4.2 Chemicals/Reagents

The precursor chemicals used for the film preparation, as well as their source and percentage purity are listed as follows:

- Cadmium sulphate Cd SO_4 (Percentage purity = 99%): it is used as cadmium ion.
- Thiourea CS $(N\ H_2)_2$ (Percentage purity = 99.0%): it is used as sulfur ion.
- Ammonia solution: as the complexing agent.
- Distilled water: as the solvent.
- Nitric acid: for cleaning the substrates, magnetic stirrers and beakers.
- Alcohol: for cleaning the substrates.

3.4.3 Substrate cleaning procedures

Substrate cleaning is the process of breaking the bond between the substrate and contaminants. Due to the variety of processes involved in manufacturing substrates, extreme cleanliness is required to remove common contaminants such as dust particles, some adsorbed water and other debris. Glass substrates were used for film deposition. Substrate cleaning plays an important role in forming smooth, uniform, and adherent films. After washing the glass substrate with ordinary water and soup, it was immersed in nitric acid for 24 hours. These were washed with fresh water and immersed in ethanol alcohol for 30 minutes. They were then washed with clear distilled water and air dried.

3.4.4 Reagent's Solution Preparation

The reagents solutions are prepared individually as follows,

3.4.4.1 Preparation of 0.1M aqueous cadmium sulphate

Using a beam balance, measure 7.618 grams of cadmium sulphate. The mass of cadmium sulphate is calculated by multiplying the concentration in moles, the volume in liters, the molar weight in grams, and the percentage purity in percent.

Cadmium sulphate was weighed into a beaker. The salt was dissolved in small amount of distilled water and then transferred into100 ml volumetric flask using funnel. The solution was then topped up to the 100 ml mark with distilled water. The concentration of the resulting solution was 0.1M.

3.4.4.2 Preparation of 0.2M of thiourea

Using a beam balance, measure 1.507grams of thiourea. The mass of thiourea is calculated by multiplying the concentration in moles , the volume in liters, the molar weight in grams and the percentage purity in percent. Thiourea was weighed into a beaker. The salt was dissolved in small amount of distilled water and then transferred into100 ml volumetric flask using funnel. The solution was then topped up to the 100 ml mark with distilled water. The concentration of the resulting solution was 0.2M.

Figure 4: Sample image of Reagent's Solution Preparation

3.4.5 Preparation of cadmium sulphide thin film

Numerous trials were conducted to optimize the deposition parameters for obtaining high-quality CdS thin films. After parameter optimization, the actual mother solution was prepared by sequentially adding the following precursor solutions:

The first sample was prepared by mixing 5 ml (0.1 M) of cadmium sulphate aqueous solution as precursor concentration, 10 ml distilled water, 5ml of ammonia solution as complexing agent ,5 ml (0.2 M) thiourea and 25 ml of distilled water, with a total volume of 50 ml. The prepared glass substrate was immersed in the solution, which was then placed in a water bath at 40°C for 30 minutes. Initially, the solution's color was white, but after 7minutes, it began to change to yellow. Subsequently, a thick, glossy, adherent, yellow cadmium sulphide (CdS) thin film was deposited.

The thin films were washed with distilled water to remove any precipitates, air-dried, and finally annealed at 30^0Cfor 1 hour and 30 minutes. The thin film also coated the surface of the cup, changing the color to yellow and enhancing its appearance.

A second sample was prepared by mixing 5 ml (0.1 M) of cadmium sulphate aqueous solution as precursor concentration, 10 ml distilled water, 5ml of ammonia solution as complexing agent ,5 ml (0.2 M) thiourea and 25 ml of distilled water, with a total volume of 50 ml. The prepared glass substrate was immersed in the solution, which was then placed in a water bath at 50°C for 30 minutes. Initially, the solution's color was white, but after 7minutes, it began to change to yellow. Subsequently, a thick, glossy, adherent, yellow cadmium sulphide (CdS) thin film was deposited. The thin films were washed with distilled water to remove any precipitates, air-dried, and finally annealed at 30^0Cfor 1 hour and 30 minutes. The thin film also coated the surface of the cup, changing the color to yellow and enhancing its appearance. The third, fourth, and fifth samples were deposited in the same manner as the second sample, with only a 10^0C variation in temperature. Figure 5: illustrates the formation of pure CdS thin films.

(A) First solution at 0 minute (B) Final solution at 30 minute

Figure 5: Photo images of the deposition process of CdS thin films mother solution as deposition time increase from 0 to 30 minutes at 80^0C.

(A) First sample of thin film at 40^0C. (B) Final sample of thin film at 80^0C

Figure 6: Photo images on pure CdS thin films on the substrate at 40^0C and 80^0C.

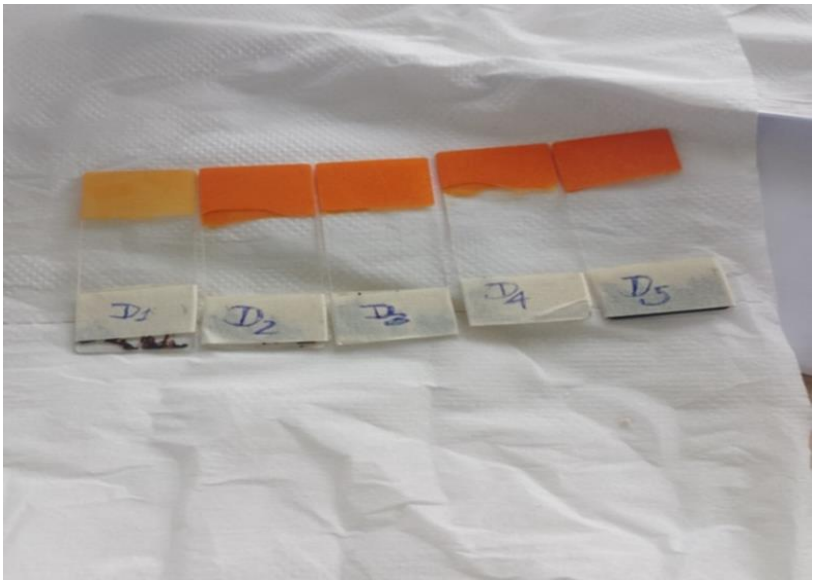


Figure 7: Sample images of CdS thin films.

3.4.6 Characterization techniques used

Sample characterization is an integrated process with thin film deposition. Different techniques were used for the characterization of the thin films. Structural characterization of the CdS thin films was carried out by using the XRD-7000 x-ray diffractometer operating at 30 kV and 40 mA with Cu Kα monochromatic radiation (λ=0.15406 nm) in the Bragg-Brentano geometry and optical properties were studied by measuring the absorbance of the thin films at room temperature using a T80 UV/VIS Spectrometer.

CHAPTER -FOUR

4. RESULT AND DISCUSSION

4.1 Optical Studies of CdS thin films

4.1.1. Optical absorption

The optical properties of the CdS thin films were analyzed by measuring their absorbance within the 400-800 nm wavelength range using a T80 UV/VIS spectrophotometer. Figure 8: displays the absorption spectra of the films, demonstrating the influence of deposition temperature. The absorbance spectra reveal a smooth decrease from UV to near-IR region. Materials exhibiting wavelengths below 520 nm, such as CdS, possess a strong absorption coefficient, making them well-suited for solar cell applications. This suggests that CdS thin films effectively absorb light in the desired range. The first sample, in particular displayed both high absorbance and high energy band gap. This observation highlights an important relationship with significant implications. As direct band gap semiconductor, CdS exhibits enhanced absorbance at wavelengths corresponding to its high energy band gap, facilitating direct electron transitions. The coexistence of high absorbance and a high energy band gap underscores CdS's potentials in advanced optoelectronic devices like solar cells, photo detectors, and LEDs, where efficient light absorption and precise band gap control are critical.

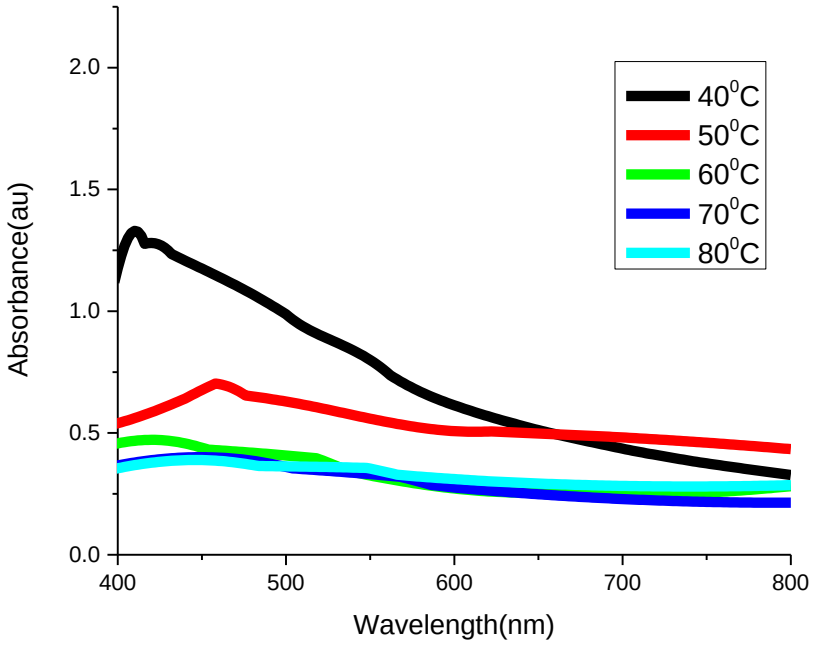


Figure 8: Absorbance versus wavelength graph of CdS thin film obtained at different temperature.

4.1.2. Optical band gap

The optical band gap of the thin film was estimated from data obtained from optical absorbance versus wavelength with the Stern (1963) relationship of near-edge absorption which is given as [33]:

$$A = \frac{[K(h\nu - Eg)]^{\frac{n}{2}}}{h\nu} \quad \text{..... (4.1)}$$

Where A is the absorbance, Eg is the band gap, v is the frequency, h is the Planck's constant, k is a constant while n carries the value of either 1 or 4. The value of n is 1and 4 for the direct transition and indirect transition, respectively. CdS is a direct band gap material, thus n is taken as 1. The band gap energy was determined by extrapolating the linear portion of $(Ahv)^2$ versus hν to the energy axis at $(Ahv)^2 = 0$ .The band gap energies of the CdS thin films were found to be 1.80 eV , 1.76V, 1.70 eV , 1.66 eV and 1.37 eV at deposition temperatures 40^0C, 50^0C, 60^0C, 70^0C,and 80^0C, respectively. This indicates that the higher deposition temperatures significantly affect the direct band gap. The results show that the band gap energy decreases with increasing deposition temperature.

This suggests that at higher temperatures, the CdS thin films have smaller band gap, making them more conductive and better at absorbing light. Conversely, at lower temperatures, the band gap is larger, indicating lower conductivity and reduced light absorption capacity. The variation in the band gap energy could be useful for designing suitable absorber materials for solar cell fabrication.

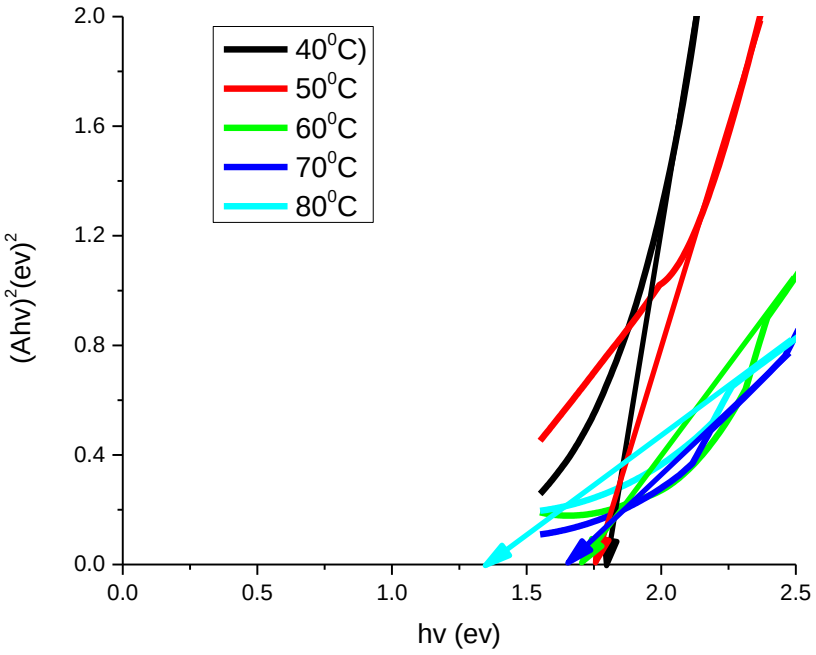


Figure 9: Plot of (Ahv) ^{2} versus hv for five samples of CdS thin film obtained at different temperature.

Table 3: Variation of direct band gap energy with five different deposition temperatures of cadmium sulphide thin films.

Deposition temperature	Band gap (ev)
40^0C	1.80
50^0C	1.76
60^0C	1.70
70^0C	1.66
80^0C	1.37

In general, when the deposition temperature increases, the band gap energy of the deposited materials generally decreases. This is because a higher temperature provides more energy to the atoms, allowing them to rearrange and form a more ordered crystal structures with fewer defects. The reduction in defects and the changes in the materials composition and phase can lead to a narrowing of the band gap energy.

4.2 Structural Characterization

Structural analysis is one of the most common techniques used in the characterization of thin films. X-ray diffraction is an extremely important technique in the field of material characterization for obtaining information on an atomic scale from both crystalline and non-crystalline (amorphous) materials. It can be employed to determine the phase content in many minerals and materials. The structural characterization of the CdS thin films was carried out using the XRD-7000 x-ray diffractometer with CuKα (1.5406 Å) radiation operating at 30mA and 40 kV. The CdS thin films deposited at 40^0C exhibited an amorphous structure, lacking a well-defined crystalline arrangement. However, the thin films deposited at 50^0C, 60^0C, 70^0C and 80^0C exhibit five peaks. These diffracted peaks are indexed as the (002), (101), (110), and (112) planes corresponding to angles of 26.6024, 29.00, 44.04, and 51.84, respectively at an angle 2θ. The diffracted planes align well with JCPDS card No: 41-1049 of hexagonal crystal structure and (200) planes corresponding 31.72 at an angle 2θ. The diffracted planes align well with JCPDS card No: 10-0454 cubic crystal structure. XRD results indicate that as the deposition temperature increased, five peaks appeared. This could be attributed to the enhancement of the crystal size with temperature. It is also observed that the preferred orientation of the crystal was along the (002) plane, which is a densely packed plane in the hexagonal structure for the sample. The intensity of the sharp peak indicates that the sample is highly crystalline.

The presence of multiple peaks , including the (101),(110), (112) planes for hexagonal crystal structure and (200) plane for cubic crystal structure , suggests that the CdS thin films possess a well- developed ,with various orientations presents, rather than a single orientation.

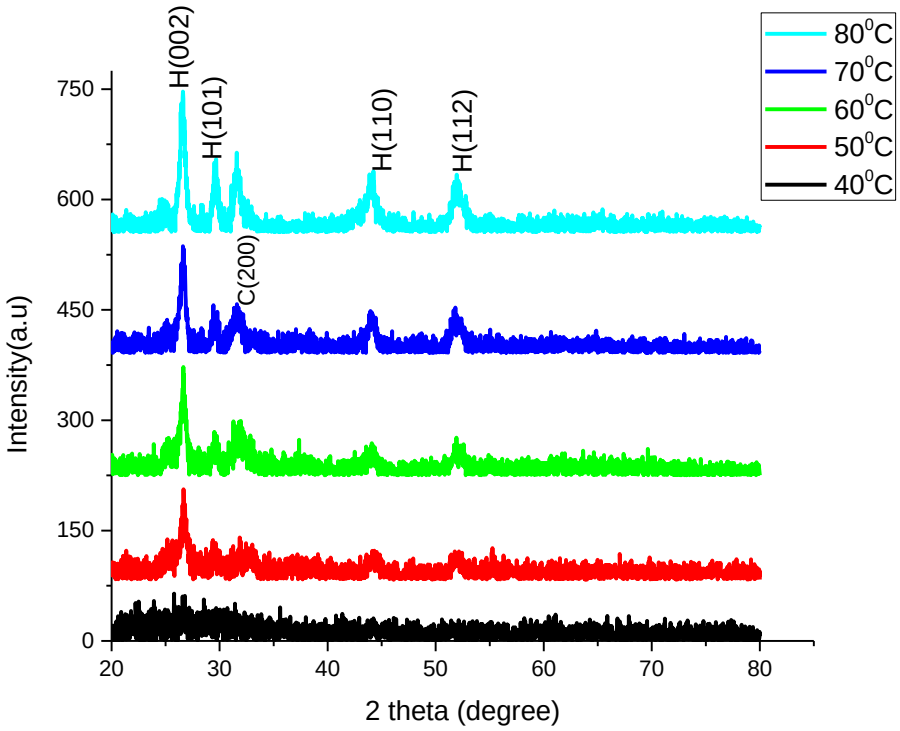


Figure 10: X-ray diffraction patterns for CdS thin films grown with five different bath temperatures deposited for 30 minute.

The crystallite size was calculated using Debye- Scherer's equation as shown in equation:

$$D = \frac{K\lambda}{\beta \cos\theta}$$

Where K is a Scherer's constant usually (K = 0.9), λ is the wavelength of X-ray (1.54060 Å), β is the full width at half maximum, FWHM in radians and θ is the angle of incidence in degree.

Mathematically, the micro strain value ε was evaluated by using the following formula :

$$\varepsilon = \frac{\beta \cos\theta}{4}$$

Where θ is the Bragg angle in radian. The dislocation density δ which is a measure of the defects in the crystallite has been calculated by using formula:

$$\delta = \frac{n}{D^2}$$

Where n is a factor, which equals unity giving minimum dislocation density and D is the crystallite size[1].

Table 4: The crystalline parameters obtained from XRD pattern for CdS thin films deposited on glass substrate at five different bath temperatures.

Temperature	(hkl)	Peak position 2θ(◦)	FWHM[β]	Grain size D(nm)	Dislocation Density $\delta(\times 10^{15}(lines/m^2))$	Micro strain $\varepsilon(10^{-3})$
40^0C	-	-	-	-	-	-
50^0C	002	26.65473	0.85395	9.05	12	3.6
60^0C	002	26.62027	0.68187	11.34	8	2.9
70^0C	002	26.5891	0.64797	11.93	7	2.8
80^0C	002	26.57419	0.60054	12.87	6	2.6

As we have seen from this table, as the bath temperature increases from 50^0C to 80^0C, the crystallite size increases. This is because a higher temperature provides the atoms with more energy, allowing them to move freely and form large, more stable crystalline structures.

CHAPTER- FIVE

5. CONCLUSION AND FUTURE STUDY

5.1. Conclusions

In this work, the CdS nanocrystalline thin films were successfully deposited using the CBD method on the glass substrate at five different bath temperatures. Various characterization techniques were employed, leading to the conclusion that deposition temperature plays a crucial role in the synthesis of these thin layers. Optical band gap studies conducted on the deposited CdS thin films after 30 minutes revealed a decrease in the optical band gap from 1.80 eV to 1.37 eV as the temperature increased from 40^0C to 80^0C. This indicates an inverse relationship between deposition temperature and band gap energy of CdS thin films, suggesting that higher deposition temperatures lead to CdS thin films with smaller band gaps, resulting in increased conductivity and light absorption capabilities. XDR analysis showed the deposited CdS thin films exhibited a simple hexagonal crystal structure with preferred orientation along the (002) plane. The intensity of the sharp peak indicates that the sample is highly crystalline. Additionally, the crystalline size of the CdS thin films increased with higher bath temperatures.

The effect of deposition temperature on the structural and optical properties of cadmium sulphide thin films is clear. With increasing the effect of deposition temperature, band gaps decreased and grain sizes increased.

5.2 Future study

Further investigations are needed:

1. To investigate the effect of bath temperature on morphological and electrical properties of CdS thin films.

2. To study the effect of thiourea concentration on morphological, electrical, optical, and structural properties of CdS thin films.

3. To investigate the effect of deposition time on the thickness, optical, electrical, morphological, and structural properties of CdS thin films at different pH value.

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