

Investigation of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ and CdMgS Thin Films for Energy Conversion Material Using Experimental and Theoretical Approaches



Ahmed Umer Yimamu

A PhD Dissertation Submitted to the Department of Applied Physics,

College of Applied Natural Science

Presented in a Partial Fulfillment of the Requirement for the Degree of

Doctor of Philosophy in Applied Physics (Material Physics)

Office of Graduate Studies

Adama Science and Technology University

December, (2024).

Adama, Ethiopia

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Adama, Ethiopia

Declaration

I declare that the author of this dissertation, which is titled **Investigation of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ and CdMgS Thin Films for Energy Conversion Material Using Experimental and Theoretical Approaches** has not been submitted for a comparable reason to any other university. This dissertation properly acknowledges its references with appropriate citations.

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I/we, the supervisor(s) of this dissertation, hereby certify that I/we have read and revise the dissertation entitled **Investigation of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ and CdMgS Thin Films for Energy Conversion Material Using Experimental and Theoretical Approaches** prepared under my/our guidance by Ahmed Umer Yimamu submitted in the partial fulfillment of the requirements for the degree of Doctor of Philosophy in Applied Physics (specialization in material physics).

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This dissertation certifies that I/we have read and edited the dissertation and that the board of examiners' views and suggestions have been suitably integrated into the final version of the dissertation titled **Investigation of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ and CdMgS Thin Films for Energy Conversion Material Using Experimental and Theoretical Approaches** We, the undersigned, members of the Board of Examiners of the dissertation open defense by **Ahmed Umer Yimamu**, have read and evaluated the dissertation titled Investigation of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ and CdMgS Thin Films for Energy Conversion Material Using Experimental and Theoretical Approaches and examined the candidate during open defense. This is, therefore, to certify that the dissertation is accepted for partial fulfillment of the requirement of the degree of Doctor of Philosophy in Applied Physics (Specialization in **Material Physics**)

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LIST OF ACRONYMS AND ABBREVIATIONS

AD	As-deposited
CdTe	Cadmium Telluride

CIGS	Copper Indium Gallium Selenide
CV	Cyclic Voltammetry
DFT	Density Functional Theory
DI	Deionized water
ED	ED
EDS	Energy-dispersive X-ray spectroscopy
FHWM	Full Width Half Maximum
FTO	Fluorine-doped tin oxide
GGA	Generalized gradient approximation
ITO	Indium-doped tin oxide
LDA	Local density approximation
OPVs	Organic Photovoltaics
PCE	Power conversion efficiency
PEC	Photoelectrochemical cell
PSCs	Perovskite SCs
PTFE	Polytetrafluoroethylene
PV	Photovoltaics
PWSCF	Plane wave self-consistence field
PEC	Photoelectrochemical cell analysis
QDs	Quantum Dots
SEM	Scanning electron microscopy
TCOs	Transparent conducting oxides
UV-Vis	Ultra violet visible Spectroscopy
XRD	X-ray Diffraction

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Abstract

Cadmium telluride (CdTe), Cadmium zinc telluride (CdZnTe), and Cadmium magnesium sulfide (CdMgS) thin films were generated in an acidic aqueous solution utilizing a low-cost two-electrode (TE) electrodeposition (ED) technique. The CdTe thin films were synthesized at various cathodic voltages to investigate the deposition voltage range from (1200 -1450) mV with a 50 mV raise. The structural, optical, and Photoelectrochemical cell study shows that the film deposited at 1250 mV will be taken as optimized voltage. CdTe thin films were synthesized at different deposition pHs, such as 1.8, 2.5, 3.0, and 3.5. According to the structural study, the deposited CdTe thin films feature mixed-phase hexagonal and cubic zinc blend structures in their as-prepared (AD) and annealed (HT) forms, with pH depositions of 1.8, 2.5, and 3.5. When the pH of the depositing reaches 3.0, only a single-phase cubic structure is visible. The maximum crystallite size is 23 nm HT samples for conforming pH values 3.0. For AD samples, the energy bandgaps were measured (1.38 - 1.58) eV, and for HT (1.35 - 1.5) eV, for a range between (1.8 - 3.5) pH values. The entire outcome demonstrates that a CdTe film of high quality for solar cell (SC) usage was formed at a pH of 3.0. The structural study reveals that CdZnTe thin films are cubic structures. The band gap of CdZnTe was increased from (1.82-2.12) eV for AD samples and (1.52-1.74) eV for HT samples with (0.25-1.00) M Zn concentrations, respectively. The structural analysis of CdS: Mg verified the formation of hexagonal films. The CdS: Mg thin films had the least surface morphology at a deposition voltage of 1450 mV. When the cathodic voltage was used between (1445 -1465) mV, the energy band gap of CdS: Mg thin films was in the range (2.44 - 2.47) eV. Results from Raman spectroscopy exhibited that the first longitudinal optic (1LO) phonon vibration revealed a high peak at 306 cm^{-1} wave number. With the possibility of being used as a buffer layer in thin-film CdTe-based SC systems, the film deposited at 1450 mV demonstrated the best quality. CdZnTe structural optimization, state density, and electron energy band structure are studied using DFT. The optical spectra of CdTe and CdZnTe are calculated, including the real and imaginary parts of dielectric parameters, energy loss functions, absorption coefficient, reflective index, and conductivity, and the analysis confirmed that the values varied with Zn- concentration.

Keywords

CdZnTe, CdTe, CdMgS, Two-electrode, ED, Zn-concentration, deposition parameter

1. Introduction

1.1. Background

A promising approach to the world's energy issue has been using solar energy (SE) to generate electricity. A SC is a device that utilizes sunlight to produce electricity (Lee & Ebong, 2017). The cost of producing solar panels is one of the significant difficulties in employing this energy source, as well as conversion efficiency, lifetime, and stability problems. The affordability of this device is impacted by the high cost of synthesis and manufacture associated with the leading Si-based SCs on the market today (Akande et al., 2023). The alternative to extracting this significant energy from the sun is thin film-based SCs, which use inexpensive materials synthesis and production techniques. In order to address such problems, growth techniques such as low-cost TEED techniques and energy conversion materials play a great impact. Chalcogenides compound group II-VI semiconductors materials based on cadmium and zinc (CdS, CdTe, CdSe, ZnS, ZnSe, ZnTe) have been widely employed in the manufacturing of solar devices based on thin films (Keser & Peksoz, 2020).

Because of its special qualities, including its high absorption coefficient, direct energy band gap, which is close to the optimal band gap for absorber material (1.5 eV), low-cost deposition techniques that can deposit it, and growth with either n- or p-type conductivity, the CdTe-based SC has drawn the attention of numerous research groups to lower the cost of production (Oluyamo et al., 2021a), high theoretical conversion efficiency (33%)(Shi et al., 2019), simple manufacturing (Fthenakis et al., 2020) and shortest energy payback time (Walker et al., 2022). CdTe's high binding energy of 6 eV per atom and melting temperature of 1041 °C are what give it its stability (Chavan et al., 2022). The Shockley-Queisser limit indicates that CdTe has an ideal band gap of around 1.5 eV, which enables it to attain efficiencies of roughly 32% at open circuit voltages more than 1 V and short circuit current densities greater than 30 mA/cm² (Rühle, 2016). The semiconductor CdTe has a bandgap that is nearly ideal for absorbing sunlight and has high electrical conductivity. The strong charge-transport, high resistivity (10⁹ Ω), high density (5.85 g/cm³), and atomic number (Cd: 48 and Te: 52) (Oluyamo et al., 2021b). Because of this, CdTe is regarded as one of the semiconductors with the most tremendous potential for thin-film SE (Mazur et al., 2023). It has been determined that the existence of imperfections in the CdTe light

absorber substantially significantly influences the photovoltaic routine characteristics of CdTe-based SC devices (Mathur & Singh, 2020).

CdTe has potential requests, including countless types of semiconductor devices like sensors (Shams et al., 2020), medical imaging (Meriuts et al., 2022), and X-ray and γ - ray detectors (Maslyanchuk et al., 2021). Thin film low-cost SC devices are getting attention nowadays due to reducing the production cost and increasing affordability of SCs. CdTe-based thin film SCs have the second market of the world's SCs next to crystalline Si-based SCs. Significant progress has been observed in the efficiency of thin-film SCs based on CdTe, especially when CdTe forms heterojunctions with window layers such as CdS, ZnS, and ZnTe (Oluyamo et al., 2021b).

The physicochemical properties of CdTe thin films and the growth circumstances during synthesis significantly influence determining their uses. CdTe thin films may be synthesized using a variety of growing processes. These techniques include Physical vapor sublimation (PVS) (Danielson et al., 2023), chemical molecular beam deposition method (CMBD) (Razykov et al., 2017), successive ionic layer adsorption and reaction (SILAR) (Samanta et al., 2017), chemical bath deposition (CBD)(Surabhi et al., 2021), physical vapor deposition(Yavorskyi et al., 2019), metal-organic chemical vapor deposition (MOCVD) (Oklobia et al., 2022a), pulsed laser deposition (PLD) (Wang et al., 2021), vacuum evaporation (Kumari, Suthar, Himanshu, Kumari, et al., 2022), co-precipitation (Golsefidi et al., 2016), spray pyrolysis (Arce-Plazaa et al., 2017), RF sputtering(Doroody et al., 2021),sol-gel (P. Zhang et al., 2023) and ED(ED) (Olusola et al., 2020). Among the growth processes mentioned above, CSS and MOCVD use expensive vacuum techniques and highly advanced equipment. It is an abnormal phase transition from a solid to a gas state. Compared to the other approaches, the solution-based approach, like CBD, is less expensive, and the phase transition from liquid to solid state is more organic. However, this approach throws the solutions away after only one usage. In this instance, in addition to Te, which is less common, a significant amount of hazardous waste, including Cd, is produced. In contrast to the other methods, the ED approach is a better way to create CdTe thin films since it is easier to dope, less expensive, and produces less hazardous waste.

This method's additional benefit is that it can be used at low temperatures, and by adjusting the deposition settings, it is easy and reasonable to regulate the size and characteristics of the films. Its self-purification ability, extended bath lifespan, simplicity, scalability, and manufacturing ability are well-established (Surabhi et al., 2021). In CdTe, thin films were synthesized in three-

and TEED configurations. In this study, to further reduce the synthesis cost, we used a low-cost TE configuration ED method (without reference electrode) instead of the conventional three-electrode configuration (Saha et al., 2020). The TEED method has advantages such as cost minimization by removing the reference electrode system simplicity, industrial manufacturing viability, and elimination of potential metal ions like K and Ag from the reference electrode and additionally, the temperature of deposition rises to 90°C (Ojo & Dharmadasa, 2017),.

In the ED method, the properties of films are powerfully precious by the type of precursor and its concentrations. Different Cd precursors reported for the ED of CdTe thin films include cadmium chloride CdCl_2 (Salim, Patel, et al., 2015), cadmium nitrate $\text{Cd}(\text{NO}_3)_2$ (Ray & Mallick, 2013), and cadmium sulfite CdSO_4 [29]. The experimental results of three and TEED methods for all precursors show that both *n*- and *p*-type CdTe films can be grown using different cadmium sources. In this dissertation, we used a low-cost TEED approach to use weak salt cadmium acetate as a Cd precursor. To the best of our knowledge, no study has been published on the use of a potentiostatic mode in a TEED configuration with an aqueous solution containing a precursor of cadmium acetate for the formation of CdTe thin film. The CdZnTe thin films were synthesized by low-cost TEED configuration in potentiostatic mode using weak salt cadmium acetate and zinc acetate as Cd and Zn precursor, respectively by using TEED approach which has not been reported yet. Using a low-cost, previously unreported TEED technique, the CdS: Mg thin films were created using cadmium chloride (CdCl_2) and magnesium chloride (MgCl_2) as Cd and Mg precursors, respectively, with varying deposition voltages. In the realm of SCs, CdTe, CdZnTe, and CdS: Mg are highly valued because of their exceptional photovoltaic characteristics, which include advantageous band gaps and high absorption coefficients. However, the high cost of their deposition methods has been one of the main challenges in making these materials viable for large-scale production. Traditional methods, such as vacuum deposition and sputtering, are not only expensive but also require sophisticated equipment, which can significantly drive up the overall cost of production.

In this context, we are particularly drawn to the low-cost TEED method, which offers an economically viable alternative for depositing thin films of CdTe, CdZnTe, and CdS: Mg. ED is a well-established technique that allows for exact control over the homogeneity, composition, and thickness of the film. It permits the deposition of these materials directly onto conductive substrates, reducing both material and energy consumption, which can lead to a significant

decrease in the overall cost of manufacturing SCs. Moreover, the TE configuration for ED is an attractive solution due to its simplicity and low operational cost. Unlike conventional methods, which often involve complex setups with multiple electrodes and higher voltage requirements, the TE system offers a competent and cost-effective way to deposit thin films while maintaining the high quality needed for SC efficiency. Integrating this method into the fabrication of CdZnTe and CdS: Mg thin films will make these materials more accessible for industrial-scale SC production.

1.2. Statement of the Problem

Semiconductor materials have an energy band gap between (0.4-4) eV, and the material's conductivity varies by changing temperature, optical absorption, and doping. They are selected as SC applications. CdTe is one of the candidates for the development of thin film SCs used as absorber material since its high absorption coefficient, direct band gap, and energy band gap of 1.45 eV, which is close to the ideal energy band gap of the absorber layer of 1.5 eV. Despite this benefit, crystalline silicon SCs continue to outperform CdTe technology.

Complements in efficiency, commercialization, and consistency. This is because of impurity in the growth of CdTe during growth, grain boundary, lack of good junction partner, back contact stability, and other defects.

Reducing absorption loss in the buffer layer and lattice-mismatched contributed substantially to creating thin-film SCs based on CdTe. This study focuses on the properties of thin film CdTe: Zn absorber material used for SC technology. To increase the efficiency of CdTe/CdS thin film SCs by raising the carrier lifetime, decreasing recombination, and increasing mobility by doping and CdTe thin film absorber material for SE conversion.

To improve the above parameters, we must study the structural, morphological, electronic structure, and optical properties of CdTe: Zn thin film by ED using the doping and density functional theory (DFT) method. The effect of deposition voltage on CdS: Mg thin films by utilizing a low-cost TEED approach.

1.3 Objective

1.3.1 General Objective

The main objective of this study is to investigate the structural, morphological, electronic structure, and optical properties of CdTe, CdTe: Zn, and CdS: Mg doping thin films deposited using ED method and DFT study for SE application.

1.3.2 Specific Objective

The specific objectives of this dissertation are to

- ✓ Optimization of the deposition pH for CdTe using a low-cost ED method.
- ✓ Examine deposition parameters for CdTe: Zn thin films and CdS: Mg doping deposition, deposition voltages (Vg).
- ✓ Determine optical absorption enhancement of (Zn) doped CdTe thin film growth using the ED method.
- ✓ Analyze the effect of Zn and Mg dopants on optical properties, in particular, the effect of concentration on band gap engineering and electronic structure of CdTe and CdS thin film.
- ✓ Explain the effect of CdTe: Zn doping on the electronic structure using DFT.

1.4 Significance of the Study

Energy is one of the primary driving forces for technology development and industrialization. It is the first of the top ten hot research issues worldwide. Fossil fuels are one of the dominant sources of energy. They are limited resources, not environmentally friendly, and can seriously affect our health and environment. SE is the preferred one to solve this problem because of its unlimited resources, is environmentally friendly (green technology), and is available on the surface of the earth, having a higher potential for use in the future.

There are three parameters that can be taken into consideration when using this energy: material cost, efficiency, and lifetime. SE material, which is a compound semiconductor CdTe thin film, is one of the best absorber layers. CdTe will be deposited using a low-cost ED method, and we can improve the structure using doping mechanisms. Morphology and optoelectronic properties of the film are needed for better efficiency and lifetime.

Some of the significance of this study is that using the ED method for the growth of CdTe thin film for SC application includes low cost, simplicity, scalability, and Cd-containing waste reduction will be used as an advantage. This study will contribute significantly to developing thin film CdTe, deposited using the low-cost TEED method for SC application using a doping mechanism.

1.5. The Dissertation's Layout

This study covers ED of CdTe, CdZnTe, and CdMgS thin films in low-cost TE systems with a potentiostatic approach and density functional study of these compounds by using a quantum espresso package. This dissertation contains five chapters. Chapter one deals with a general

introduction to renewable energy sources, the objectives and significance of the study, and the thesis layout. Chapter two deals with a review of the literature and a detailed explanation of the development of thin film SCs, the working principle of thin film SCs, and their components. Chapter three covers materials used, experimental synthesis methods, and computational methods. Chapter four covers the main findings and data analysis part. Chapter Five lays out the conclusions and recommendations part of the study.

2. Literature Review

2.1. Introduction

The need for energy facilities will expand due to population growth, financial expansion, and industrial improvements, while the demand for main energy will rise by 1.3% year until 2040 (Worku et al., 2024); (Mozakka et al., 2022). Fossil fuels dominate the world's energy supply, and the grim fact of escalating climate change necessitates an expedient switch to clean, efficient energy sources (Lohani et al., 2023). Energy is necessary for human survival (such as food, power, etc.). Fossil fuels, including coal, oil, and natural gas, remain the primary energy source today. The world's economy and population are expanding exponentially, which has led to a constant rise in energy consumption and the production of fossil fuels. There is a limited amount of fossil fuel available on earth and will ultimately run out. Moreover, the greenhouse effect has made global warming inevitable due to the emission of CO₂ waste gas that results from the combustion of fossil fuels. We must create green energy instead of fossil fuels for the benefit of coming generations of humans and to save the planet where we must all dwell.

An energy shift away from fossil fuels and toward cleaner sources is necessary for sustainable development. Energy from renewable sources, which is expected to have fewer adverse environmental impacts, is the main component of this transformation (Gayen et al., 2024; (Osman et al., 2022).

The dominant renewable sources are solar, wind, hydropower, geothermal, and biomass. Each renewable energy source has unique benefits, and the decision of whom to employ often depends on local conditions, energy needs, and environmental considerations. The advantages and disadvantages of these sources are listed below.

2.1.1. Wind Energy

Wind energy is the most advanced and established renewable energy source. It uses wind energy, which is clean, renewable energy that also lowers greenhouse gas emissions and protects the environment, to create electricity. The force of air currents creates wind energy. The benefit of wind energy is that wind turbines create power without releasing greenhouse gases. Cost-effective wind power has become one of the cheapest sources of electricity. Wind farms can be situated on agricultural or multi-use lands, allowing for dual use. Wind energy has several disadvantages despite its many benefits.

Here are some key drawbacks of wind energy generation that depend on wind speed, which can be inconsistent and unpredictable. This intermittency can affect the reliability of wind power as a continuous energy source. Wind turbines generate noise from their rotating blades and mechanical components. For those who live close, this loudness may be an issue that lowers their standard of living. Wind turbines are often large and can be visually intrusive, particularly in scenic or natural areas. This can lead to resistance from local communities and impact land values. It takes a lot of acreage to plant wind farms, which can affect land use and lead to conflicts with other land uses, such as cultivation or protection areas. However, the land around turbines can still be used for other purposes, such as farming. Practical energy preservation options are often needed to address the variability in wind speeds. These can be costly and are still developing in terms of technology and scalability.

2.1.2. Hydropower

Water is not wasted in the process of turning falling water's energy into electricity. The sun, which powers the water cycle, is basically the source of hydropower energy. The advantage of hydropower plants is that they can provide a steady and reliable energy source. It generates electricity with very low greenhouse gas emissions. Can offer energy storage through pumped-storage hydropower, balancing supply and demand. Reservoirs created by dams can help with flood control and irrigation. Hydropower, while a well-established and significant source of renewable energy, has disadvantages:

The construction of dams and reservoirs can disrupt local ecosystems, affecting plant and animal species. It can lead to habitat loss, changes in river flow, and alterations in sediment transport.

Dams can impede the natural migration of fish and other aquatic species, potentially leading to declines in fish populations and affecting biodiversity. Large-scale hydropower projects often require the flooding of large areas, which can displace local communities and disrupt their lives and livelihoods. This can lead to social and economic challenges.

2.1.3. Geothermal Energy

Geothermal energy is the earth's heat-derived energy. Near the earth's surface, high ground temperatures exist, and they are frequently close to geologically active regions that have naturally occurring hot springs. The steam generated power and was recycled back into the ground in the opposite production line. The earth's heat is constant, and water is obtained from rain and regenerated independently. The advantages of geothermal energy are that it provides a continuous

and stable energy supply. Produces very little greenhouse gas emissions and high efficiency in converting heat to electricity. Geothermal plants require less land compared to other power plants. Geothermal energy has several advantages but also comes with certain disadvantages.

Here are some of the key drawbacks, such as geographical limitations: Geothermal energy resources are location-specific and are most effective in areas with significant geothermal activity, such as tectonic plate boundaries. This limits the geographic availability of geothermal power plants. High initial costs are high for geothermal energy projects, including exploration, drilling, and plant construction. The investment required can be substantial, although operational and maintenance costs are typically lower. Heat depletion if geothermal reservoirs are not managed properly, the heat extraction rate can exceed the rate of heat replenishment, leading to a reduction in energy output over time. This requires careful management and monitoring. Environmental impact surface disturbance: The development of geothermal plants can lead to surface land disturbance and alteration of the landscape. Drilling and extraction processes can also impact local ecosystems

2.1.4. Biomass Energy

This energy is derived from biological resources, namely plant and animal components, and it is a renewable energy source. Sunlight energy is stored in biomass through photosynthesis; plants absorb SE and transform it into chemical energy. The advantages of biomass are that it reduces waste materials and organic matter that would otherwise decompose. The CO₂ that plants collect during growth balances the CO₂ that is emitted during decomposition. It can be used for electricity generation, heating, and as a biofuel for transportation.

Biomass energy has several disadvantages despite its benefits. Here are some key drawbacks of competition with food production: Food production may be hampered by the competition from crop cultivation for biomass, which might result in scarcity and increased costs. Unsustainable biomass harvesting can contribute to deforestation and loss of biodiversity. Although biomass is considered carbon-neutral over the long term, its combustion releases carbon dioxide and other pollutants. Additionally, if biomass is not sustainably sourced, it can result in higher net emissions. Biomass energy conversion can be less efficient compared to sources of green energy, such as wind or solar power.

2.1.5. Solar Energy (SE)

SE is the energy that the sun emits or produces. It involves absorbing photons from the sun and turning them into electrical energy. The energy never runs out since its source is renewable. The energy supply is never fully depleted. The advantage of the sun is that it provides a virtually limitless energy source. Solar panels can reduce or even eliminate electricity bills. Solar panels require little upkeep after installation. Produces no pollutants or greenhouse emissions when in use.

SE, while a robust and growing renewable resource, does have a disadvantage. Due to weather and the time of day, sunshine, which is necessary for solar power generation, might fluctuate. This intermittency can affect the reliability of SE as a sole power source.

Due to the high storage costs to manage the variability in SE, effective energy storage solutions like batteries are needed. These can be expensive, and the technology for large-scale energy storage is still developing. Large-scale solar farms require significant amounts of land, which could impact land use for other purposes or natural habitats, particularly in densely populated or ecologically sensitive areas. Raw materials must be extracted and processed in order to produce solar panels, which may have an effect on the environment. Furthermore, the production process may need much energy.

Solar panels can degrade over time, which reduces their efficiency and output. Typically, panels have a lifespan of 25-30 years, but their efficiency can decrease slightly each year. Solar panels need to be disposed of or recycled. This process can be challenging and costly, and improper disposal can lead to environmental issues due to the presence of hazardous materials in the panels. Behind this, SE is promising and has much energy. Our solar system would not be working without this source. Additionally, radiation from the sun indirectly promotes the creation of waves, wind, and bioenergy. The main target for this study is SE conversion materials. The following section will explain in detail the solar as an energy source.

2.2. Sunlight as the Primary Energy Source

One kind of electromagnetic radiation that the Sun emits is called solar radiation. Numerous types of energy may be created by capturing and transforming this sort of energy. There is a large range of light wavelengths in the solar spectrum. It is made up of visible light, ultraviolet (UV) light, and infrared (IR) light (E. Hossain, 2023). As shown in figure 2.1, the regions of solar spectra.

Every hour, the Sun emits around 430 quintillion Joules of energy into Earth. This is far more energy than the 410 quintillion Joules that people use annually. Therefore, if SE could be fully

used, it would be enough to meet the world's energy demands and even save some energy for unexpected events. SE is the most accessible type of renewable energy. At a rate of 3.8×10^{23} kW, the sun emits SE, of which Earth absorbs 1.8×10^{14} kW (Gayen et al., 2024).

The two main energy types that sunlight emits onto earth are heat and light. Photovoltaic (PV) cells are primarily used to harvest solar light energy, and concentrated solar power (CSP) technologies are used to gather solar heat energy.

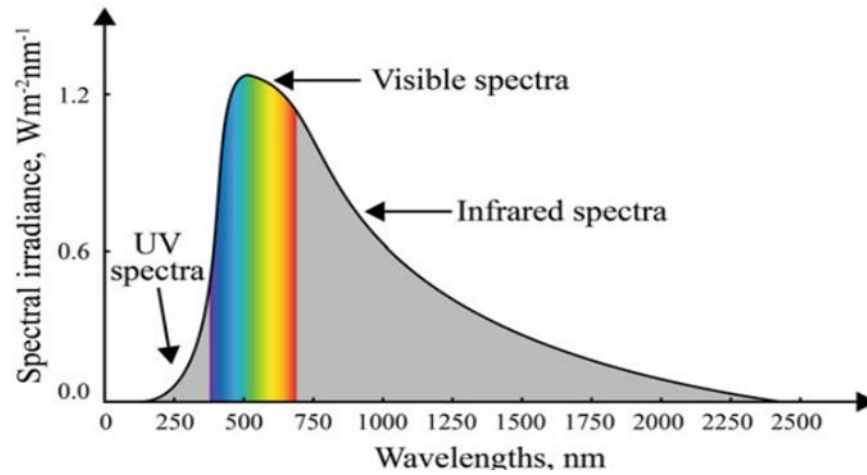


Figure 2. 1. The UV range, visible range (400–700 nm), and infrared range are the first three ranges in the solar spectrum (E. Hossain, 2023).

The device known as the SC is responsible for converting SE straight into electrical power via a technique called the photovoltaic (PV) effect. Using this large amount of source energy conversion materials plays a significant impact on the conversion of light to electricity. The main challenges of SE are the cost of production for solar panels, lifetime, environmental stability, and the panels' efficiency. Environmental problems like global warming and climate change drive people to seek alternative energy sources (Khatri et al., 2021). Fossil fuels derived from non-renewable sources are the primary dependable energy source globally. As global population continues to increase, so does the demand for energy. Substantial reservations have been raised by the depletion of these non-renewable energy sources and their ecological problems (Noman et al., 2024). Cleaner energy sources must replace reliance on fossil fuels for sustainable growth. Renewable energy is a crucial element of this transformation, as it promises to have fewer adverse environmental consequences (Gayen et al., 2024). An energy crisis might be an issue for the entire planet. One of the many renewable energy sources that can help address the world's energy dilemma is SE. SE is transformed into electrical energy by a SC (Kapadnis et al., 2020). PV is environmentally beneficial and can produce

electricity more cheaply (Seroka et al., 2022). The PV industry is constantly growing in response to the rising need for electricity (Liu et al., 2024). Thin film SCs' low material consumption and increasing efficiencies make them attractive options in the photovoltaics industry. Copper indium gallium selenide (CIGS), α -silicon (α -Si), and star absorber materials like cadmium telluride (CdTe) are the three most well-known thin film technologies that are currently being thoroughly investigated. A comprehensive review of SE materials encompasses the various materials used in PV systems and their properties, performance, and advancements. Here is an overview of key materials and their roles in SE technology.

2.3. Classifications of SCs

The materials and production techniques used to make SCs have a significant impact on their categorization. Although the industry is dominated by conventional silicon-based cells (monocrystalline and polycrystalline) because of their dependability and high efficiency, newer technologies like perovskite, organic, and thin-film cells have the potential to provide more affordable and adaptable solar solutions in the future.

2.3.1. Silicon-based SE Materials

Silicon is the most widely used material in SCs due to its abundance, stability, and excellent photovoltaic properties. Silicon-based SE materials are the backbone of most commercially available solar technologies. The main types of silicon-based materials used in SCs are monocrystalline silicon, polycrystalline silicon, and amorphous silicon. Below is a detailed breakdown of these materials.

2.3.1.1. Monocrystalline Silicon

Made from a single continuous crystal structure. These cells are highly efficient because the electrons have fewer grain boundaries to encounter, which allows for better electron flow. The aforementioned design also achieved a power conversion efficiency of 26.6%, close to the theoretical limit power conversion efficiency (PCE) of 29.1% for a silicon SC. The combination of interdigitated backside contacts and heterojunction technology produced this result. Solar panels are expensive because of the standstill in the fabrication prices of this technology, despite its intriguing features and high scalability for industrial and commercial usage (Seroka et al., 2022). High purity and efficiency with a uniform crystal structure. Offers the highest efficiency among silicon-based cells, typically around 25%. Widely used in residential and commercial solar panels.

2.3.1.2. Polycrystalline Silicon

Polycrystalline silicon films are made up of separate crystalline grains that are separated from one another or from the substrate by interfaces. There are widely dispersed silicon dangling bonds at the grain boundary according to research on polycrystalline silicon (Gao et al., 2024). Made from silicon crystals melted together, less pure than monocrystalline. Slightly lower efficiency (13-17%) but more cost-effective. It is commonly used in various PV panels, especially in cost-sensitive applications.

2.3.1.3. Amorphous Silicon

The a-Si: H doping capacity is not very good due to the extremely long diffusion lengths (on the order of 200 μm) in typical p - n junction SCs; minority carriers generated as a result of photo-absorption are dispersed across the p and n regions of the junction where optical absorption occurs. Minority charge carriers in amorphous silicon SCs have very short diffusion lengths (0.1 μm), making it difficult to gather minority charge carriers via diffusion alone. These factors make p - i - n diodes the standard choice for a-Si: H SCs (Dambhare et al., 2021). It is a non-crystalline form of silicon, and its performance is lower efficiency (6-10%) but flexible and lightweight. This kind of solar is used in thin-film SCs and some flexible PV applications.

2.3.2. Thin-Film Materials

Thin-film materials for SCs are an exciting class of materials used to create photovoltaic devices with very thin layers of semiconductor material. Thin-film SCs are distinct from traditional silicon-based SCs because they use much smaller amounts of material (often just a few micrometers thick) to absorb sunlight. These materials can be applied in a variety of ways, including deposition onto flexible substrates, which offers significant advantages in terms of weight, cost, and versatility for specific applications. Below are the main types of thin-film SC materials.

2.3.2.1. Cadmium Telluride (CdTe)

The semiconductor compound cadmium telluride (CdTe) belongs to the group II-VI chalcogenide family. It is a viable option for advancing photovoltaic (PV) technology using thin film SE. The second marketable SC after crystal silicon is a CdTe-based SC. Because of the special qualities of CdTe, including its high absorption coefficient, direct energy band gap, which is close to the ideal band gap for absorber material (1.5 eV), its ability to be deposited using low-cost deposition techniques, and its ability to grow with either n - or p -type conductivity, the CdTe-based SC has

(Yimamu et al., 2023b). Have a high absorption coefficient, allowing for thin layers. Performance efficiency of around 22.1 % and are used in large-scale solar farms due to their cost-effectiveness.

2.3.2.2 Copper Indium Gallium Selenide (CIGS)

CIGS cells are made from a combination of copper, indium, gallium, and selenium, which are layered on a substrate, often glass, plastic, or metal. Alloying the ratio of indium to gallium can be adjusted to optimize the efficiency and performance of the cell. High flexibility and absorption make them appropriate for various uses, such as photovoltaics incorporated into buildings.

Efficiency of about 15-22%. Suitable for both flexible and rigid panels. CIGS cells can still be more expensive to produce than conventional silicon cells.

2.3.2.3. Organic Photovoltaics (OPVs)

Organic photovoltaics (OPVs) are a type of SC that uses organic compounds to change sunlight into electricity. PVs are made from carbon-based materials, typically small organic molecules or polymers. Power efficiency (typically 8-12%) but offers flexibility and low manufacturing costs.

2.3.3. Emerging and Advanced Material

2.3.3.1. Perovskite SCs

Perovskite SCs (PSCs) are an innovative type of SC that utilizes a perovskite-structured compound as the light-harvesting active layer. Because of their tremendous efficiency, they have attracted a lot of attention, have low production costs, and have ease of fabrication in contrast to conventional SCs made of silicon. The material's typical perovskite structure has a formula of ABX_3 . PSCs have the amazing benefit of being compatible with both first- and second-generation SC technologies, which opens up a world of possibilities. In order to explore the unrealized potential of high-performing PV cells, perovskite materials can be coupled with traditional SCs like silicon and CIGS to construct cohesive tandem SCs (Noman et al., 2024). High absorption and potential for low-cost manufacturing, Rapidly increasing efficiency, currently around 20-25%. While PSCs show great promise, challenges remain, including long-term stability, toxicity of some materials (like lead), and scalability for mass production.

2.3.3.2. Quantum Dot SCs

Nanoscale semiconductor particles quantum dots (QDs) have special electrical characteristics because of the quantum mechanics effect. The size of the dots can be adjusted to tune their light absorption properties, allowing for customization based on the solar spectrum. Because of their special qualities, which include a wide range of visible and near-infrared light absorption, several

excitonic effects, easy surface modification to manipulate their optoelectronic characteristics, and solution processability, QDs have garnered a lot of interest in the photovoltaics industry (Huang et al., 2024). Utilize quantum dots to absorb different wavelengths of light. Potential for high efficiency, but currently in the experimental phase. Research focuses on improving performance and commercial viability.

2.3.3.3. Tandem SCs

Tandem SCs are a type of photovoltaic technology that stacks two or more layers of SCs on top of each other, each designed to absorb different parts of the solar spectrum. This design allows for greater efficiency than traditional single-junction SCs, which can only absorb a limited range of light. By using multiple layers, tandem SCs can capture more sunlight and convert it into electricity. They can achieve efficiencies exceeding 30%, compared to around 20% for conventional cells. Common combinations include perovskite and silicon, where the perovskite Higher-energy photons are absorbed by the layer, whilst lower-energy photons are captured by the silicon layer.

Developing SE materials requires balancing efficiency, cost, durability, sustainability, and scalability. The ideal material for a given application depends on specific needs, such as high efficiency, low cost, environmental impact, and adaptability for integration into diverse systems. Efficiency is the ratio of electrical output to sunlight input. Higher efficiency means more energy is converted from sunlight. While SC efficiency varies widely by type, ongoing advancements in technology and materials push efficiency levels higher, making SE more viable and cost-effective. Cost includes raw materials, manufacturing processes, and scalability. Lower costs are crucial for broader adoption. The cost of SCs has declined significantly over the past few decades, making SE more accessible. Here is an overview of the factors influencing the cost of SCs, types of solar technologies, and current pricing trends.

Longevity of materials must withstand environmental conditions (UV exposure, temperature fluctuations) and maintain performance over time. Stability considers the lifecycle impact of materials, including resource extraction, manufacturing, use, and disposal. The field of SE materials is diverse and rapidly evolving, with ongoing research aimed at improving efficiency, reducing costs, and enhancing the environmental sustainability of solar technologies. Each material has unique advantages and trade-offs, influencing its suitability for different applications and market segments.

2.4. Developments of CdTe-Based thin film SCs

The PV effect is used to harvest electrical energy or photovoltaic energy directly from sunlight, first discovered in 1839 by French physicist Alexandre-Edmond Becquerel (Singh et al., 2021)(Buckner et al., 2016). The primary prerequisite for any material to be utilized in SCs is its capacity to transform the visible spectrum of sunlight into electrical energy. When a material absorbs photons with energy equal to or higher than its energy gap, electron-hole pairs are created (N. Sinha & Sinha, 2024). In 1972, Bonnet and Raben-horst first created CdTe SCs, which had a 6% efficiency due to a CdS/CdTe heterojunction. This kind of heterojunction has been used ever since to produce thin-film CdTe SCs (Romeo & Artegiani, 2021).

Ferekides et al. reported that CdS/CdTe heterojunction SCs use thin films. Chemical bath deposition was used to create CdS films, and close-spaced sublimation was used to manufacture p-CdTe films. A claimed AM15 efficiency of 15.8% is found in a CdS/CdTe SC covering an area larger than 1 cm² (Britt & Ferekides, 1993).

National Renewable Energy Laboratories (NREL) reported by Wu et al produced a redesigned CTO/ZTO/CdS/CdTe device structure that may be used to increase the repeatability and device performance of CdTe cells. Manufactured a CdS/CdTe polycrystalline thin-film SC with an NREL-confirmed total area efficiency of 16.5%, and they obtained a high FF of 77.34% and a high J_{sc} of over 26 mA/cm² (X. Wu R. G. Dhere, C. DeHart, D. S. Albin, A. Duda, T. A. Gessert, S. Ashar, D. H. Levi and P. Sheldon, 2001).

A revised CdTe SC device design that eliminates CdS and considers other characteristics, including copper embedding, band gap grading, and a more transparent n-layer. First Solar has produced a device with a 21.5% efficiency after these modifications (Borysenko et al., 2021). Significant advancements in materials and systems have occurred in solar photovoltaic technology in recent years, improving energy storage capacity, cost, and efficiency. Due to these developments, solar photovoltaic technology is now a more practical choice for producing and storing renewable energy (Dada & Popoola, 2023).

To advance the efficiency and performance of the CdS/CdTe-based thin film, SCs, unlike dopants, are added to the CdTe lattice to increase the energy band gap and the surface nature of the films. ZnTe is material II-VI family with a lattice constant of $a = 6.1034 \text{ \AA}$; this crystal typically has a cubic zincblende structure (M. S. Hossain et al., 2010). When these materials are made of alloy with CdTe thin film, the energy band gap will be increased, and the lattice constant is reduced.

One of the primary motivations for its investigation of CdZnTe is tunable energy bandgaps, which can produce wider bandgaps than CdTe thin films. The energy bandgap estimates fall between 1.45 eV for CdTe and 2.25 eV for ZnTe (Kathalingam et al., 2021). Benefits of CdZnTe include band gap tunability, high atomic number components, continuous stability, low leakage current, high absorption coefficient and carrier mobility, and the flexibility to modify lattice characteristics (Sharma et al., 2023; Surabhi et al., 2022; Shah et al., 2021). On the other hand, reducing the concentration of Cd toxic and adding Zn, which is a friendlier and non-toxic element. Manganese (Mn) is added to CdTe to create CdMnTe (CMT), an ED ternary compound that will be utilized as the p-type window layer in CdTe-based photovoltaic cells. Again, the strong lattice matching of MnTe with CdTe has led to the selection of Mn for incorporation (A. E. Alam et al., 2020). CdS is commonly utilized in thin-film solar panels, including CdTe and CIGS SCs, as a buffer layer or window layer (Geremew & Abza, 2020; Werta et al., 2020). CdTe/CdS-based technological improvements further enhance their efficiency, stability, and eco-friendly sustainability, expanding their applications in the renewable energy division due to its direct bandgap semiconductor with a bandgap energy of approximately 1.45 and 2.42 eV, respectively. The evolution of CdTe-based SCs has greatly benefited by advancements in window materials, back metal contacts, and front contacts transparent conducting oxide (TCO) (Bosio et al., 2018). To increase SC efficiency, research focuses on improving the morphology, crystallinity, and interface characteristics of CdS thin films. The aforementioned problems of lattice mismatch and absorption loss are the primary obstacles, particularly for window materials CdS.

Various metal components are added to the CdS lattice to enhance the characteristics of CdS thin films, such as Mn-doped CdS (Kharabaneh et al., 2021), Ni-doped-CdS (Yahia et al., 2019), Co-doped CdS (Khani et al., 2021), Ga-doped CdS (Echendu et al., 2019), Zn-doped CdS (Y. Zhang et al., 2016) (Werta, Echendu, et al., 2019), Cu-doped CdS (Nazari Setayesh et al., 2023) and F and Mg-doped CdS (Sivaraman et al., 2016) are reported in the literature. Mg was chosen as the study's target element for two reasons. The first is the tuning of optical characteristics when the bandgap of CdS thin films is changed by Mg doping. By shifting the bandgap and altering the absorption spectrum, magnesium doping can raise the band gap of CdS for window material and enhance the amount of photon energy transferred to the absorber CdTe layer, making CdS appropriate for a variety of wavelength ranges. The second aim is to enhance stability and performance. Doping with Mg can improve the stability and performance of CdS thin films under different

environmental conditions. It can reduce defects in the crystal lattice, which may enhance the film's durability and efficiency in devices. In addition to this, it reduced Cd in the film, replacing Mg, a less toxic element (T. Sinha et al., 2021). In addition to the electrochemical properties already discussed, the most prevalent element, magnesium, combines with sulfur to provide a wider energy bandgap of 4.43 eV (Werta et al., 2024).

2.5. Thin film SC components and working principles

2.5.1. Components CdTe-based thin film SC

For CdTe thin film SC devices, the superstrate arrangement is the most efficient choice. This is mostly because of the way this structure enables the successful application of the required post-deposition treatment. A CdTe-based thin-film SC has several key components, each playing a crucial role in its operation. Here, the front contact, usually an oxide layer or transparent conducting-oxide (TCO), window, absorber layers, and back metal contact, respectively, are formed (Romeo & Artegiani, 2021). The detailed explanations are discussed in this section.

2.5.1.1 Transparent conducting oxides (TCOs)

These materials (TCOs) can be deposited using various methods to create thin films. $\text{SnO}_2:\text{F}$ (FTO), $\text{ZnO}:\text{Al}$ (AZO), $\text{In}_2\text{O}_3:\text{Sn}$ (ITO), and Cd_2SnO_4 (CTO) are the TCOs that have been investigated the most (Bosio et al., 2006). For visible light and near-infrared radiation, these metallic oxides show almost or greater than 90% optical transparency, and they also have extremely strong n-type conductivity. In thin film applications, the substrate comprises over 98% of the material; therefore, selecting a low-cost material like soda lime glass is imperative to keep costs under control. Sodium and potassium, which can permeate into the device and weaken it, and the fact that the glass becomes pliable at temperatures higher than 500 °C, are the limitations of soda lime glass (Romeo & Artegiani, 2021).

TCOs are transparent in the visible light spectrum (approximately 400-700 nm), allowing light to pass through without significant absorption or reflection. High Conductivity TCOs exhibit low electrical resistivity, meaning they can conduct electricity efficiently. This is typically achieved through doping with certain elements. Durability Many TCOs are chemically stable and resistant to environmental factors like moisture and oxidation.

Optical transparency TCOs usually have a wide band gap, contributing to their transparency in the visible range while allowing them to conduct electricity. The most commonly used front contacts

are fluorine-doped thin oxide (FTO) films and indium-doped tin oxide (ITO) films on glass substrates.

FTO one of the most widely used TCOs is fluorine-doped tin oxide (FTO), whose low resistivity is mostly dependent on the amount of fluorine substituted and the high carrier concentration created by oxygen vacancies (Ching-Prado et al., 2018).

Since FTO coating is simple to deposit and can be easily incorporated into a glass production line, it is now more cost-effective than other TCOs for thin-film photovoltaic applications. Commercial FTO-coated glass is already manufactured in large volumes. Because FTO is more electrically conductive than (ITO), it is a better fit for applications requiring effective charge transport compared to ITO; FTO is less expensive overall because it is made of more affordable and plentiful materials. Because of its exceptional thermal stability, FTO can tolerate greater temperatures when being processed and used.

ITO is a widely used TCO in various electronic and optoelectronic devices, including thin-film SCs. A substrate with the combined characteristics of a transparent ITO is being sought after in the field of organic optoelectronics devices (OOED) (Shankar et al., 2022).

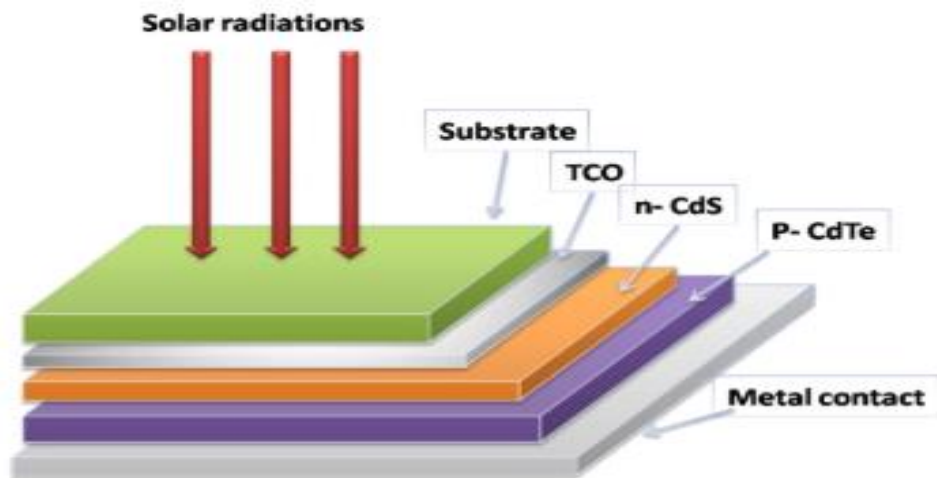


Figure 2. 2. Configuration of CdTe/CdS SC (Kapadnis et al., 2020).

It is highly transparent to visible light and has a wide band gap (around 3.5 eV), contributing to its transparency in the visible range and its conductive properties. Making it ideal for applications where both conductivity and transparency are required. It typically has a high transmittance (>80%) in the visible spectrum. In CdTe-based and other thin-film SCs, ITO is commonly used as a transparent conductive layer (front contact). It allows sunlight to pass through while conducting

the electric current generated by the cell. Indium is a relatively rare and expensive material, which can make ITO costly. Researchers are exploring alternative materials to reduce reliance on indium.

2.5.2 The CdS layer

The CdS window layer's band gap ($E_g = 2.42$ eV) prevents the entire advantage from being realized. Since the CdS window layer absorbs most of the blue photons, they effectively don't contribute to photocurrent production. To admit more photons into the CdTe absorber, CdS must thus be thinner or have its band gap increased by alloying without having to replace it entirely (Barkhouse et al., 2015). In the CdTe/CdS SC, the CdS film is called the "window layer." Its ability to form an n-type *p-n* junction with p-type CdTe is made possible by this. Because CdS has an energy gap of 2.42 eV and is transparent in the visible portion of the solar light spectrum, solar light can penetrate the CdTe layer and cause the photovoltaic effect (Bosio et al., 2006). It acts as a buffer layer and forms a heterojunction with the CdTe layer. It helps in creating an electric field that separates the generated electron-hole pairs.

2.5.3. The CdTe layer

Cadmium telluride (CdTe), an alternative to these technologies, has garnered particular interest in comparison to other materials because of its high absorption coefficient ($> 10^5/\text{cm}$) in the visible portion of the solar spectrum, great chemical stability, and ideal band gap of 1.5 eV at ambient temperature. With a lattice period of 6.481 Å, CdTe possesses a cubic zinc blende structure (Mazur et al., 2021). Moreover, CdTe has a high optical absorption coefficient, absorbing over 99% of incoming sunlight with an active thickness of around 2 μm . Having this property, CdTe can be used as an absorbed layer in thin film SCs, which is the heart of the device and the target area for this study.

2.5.4 The back-contact

Typically made from a metal such as copper, silver, or a combination of metals. Provides the electrical connection to the CdTe layer and completes the electrical circuit. It also helps reflect light back into the CdTe layer to increase light absorption. These components work together to efficiently convert sunlight into electrical energy, making CdTe thin-film SCs a popular choice for photovoltaic applications.

2.6. Working Principles of CdTe-based Thin Films SE Materials

Cadmium telluride (CdTe) thin-film SCs are a type of photovoltaic technology that converts sunlight into electricity. The intricate process of light absorption in thin films is controlled by the

interaction of many material characteristics, including refractive index, surface shape, bandgap, and film thickness. A high absorption coefficient at the appropriate wavelengths, ideal thickness, and few flaws are necessary for effective absorption. Particularly in thin-film-based systems like SCs, methods like surface texturing, light trapping, and anti-reflective coatings are crucial for increasing the light absorption efficiency. Optimizing absorption and enhancing the performance of thin-film devices requires careful material selection and device design.

Here's a basic rundown of how they work:

2.6.1. Absorption of Light

Numerous variables, such as the material's characteristics, the film's thickness, the surface shape, and the light's wavelength, affect how light is absorbed in thin films. It is essential to comprehend the fundamental mechanics of light absorption and the prerequisites for effective absorption when building thin-film devices like SCs. The absorption coefficient (α) measures a material's capacity to absorb light and is influenced by both the material's characteristics and the light's wavelength. It explains how much light is absorbed as it passes through the substance per unit distance. The absorption spectrum is mostly determined by the material's bandgap. Efficient absorption takes place when the bandgap of the material is equal to the energy of the entering photons. In semiconductor thin films, the absorption spectrum is typically limited to photon energies that are greater than or equal to the material's bandgap. The most relevant part of the light spectrum is absorbed by materials with a bandgap that is suitable for the application. For instance, cadmium telluride, or CdTe, may absorb visible light in photovoltaic applications because of its bandgap of around 1.45 eV. CdTe thin-film SC has a layer that is the primary light-absorbing material. When sunlight hits the SC, the CdTe layer absorbs photons of the visible region of the spectrum.

2.6.2. Generation of Electron-Hole Pairs

The absorbed photons transfer their energy to electrons in the CdTe material, knocking them loose from their atoms. This process creates electron-hole pairs. The electrons are the negative charge carriers, and the holes are the positive charge carriers.

2.6.3. Creation of an Electric Field

To separate these charge carriers and create a flow of electric current, an electric field is established in the SC. This is typically achieved by forming a junction between the CdTe layer and another material (usually a layer of cadmium sulfide, CdS) that has a different electronic characteristic. This junction is called a p-n junction (or a heterojunction in the case of CdTe/CdS).

2.6.4 Movement of Charge Carriers

The electric field at the junction causes the electrons to move toward the conductive layer at the back of the SC while the holes move toward the front contact. This movement of charge carriers creates a flow of electric current.

2.6.5. Current Collection

The TCO, such ITO and the back contact (a metal layer) collect the separated electrons and holes. The current is then directed through an external circuit, providing electrical power.

2.6.6. Conversion of Energy

Finally, the electrical energy generated can be pumped into the grid or utilized to power electrical devices. CdTe SCs are valued for their high absorption efficiency, which allows them to be effective even with relatively thin layers of the material. Additionally, they can be produced at a lower cost compared to traditional silicon-based SCs due to their simpler manufacturing process. Increasing the performance of CdTe-based thin-film SCs involves improving various aspects of their design, materials, and manufacturing processes. Here are some key strategies such as optimizing layer thickness, improving light absorption, enhancing junction quality, improving electrical contacts, reducing defects and impurities, advanced manufacturing techniques, increasing durability and reliability, and CdCl₂ treatment are a crucial stage in the research and development program for CdTe SCs that will significantly increase the efficiency of solar to electric conversion (I. M. Dharmadasa, 2014).

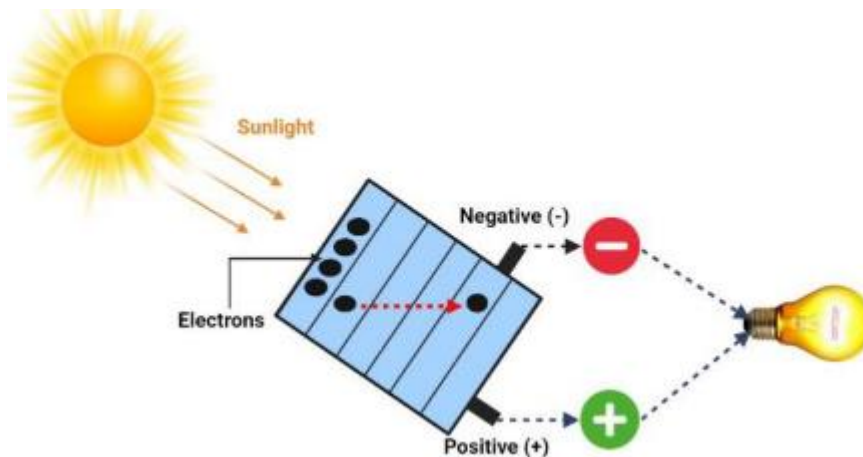


Figure 2. 3.The basic mechanisms of a normal photovoltaic cell (Khan & Jassim, 2023).

By addressing these areas, it's possible to improve the efficiency, durability, and overall performance of CdTe-based thin-film SCs, making them more competitive with other photovoltaic technologies.

The synthesis process has a direct effect on the quality, shape, and crystallinity of CdTe thin films, which in turn influences how well they work in SCs and other uses. Chemical bath deposition, sputtering, and MBE are examples of deposition processes that may produce a range of film characteristics, from high-quality, highly crystalline films to rough surfaces with poor crystallinity. Characterization methods, including XRD, SEM, AFM, and PEC measurements, enable researchers to assess the electrical, optical, and structural characteristics of CdTe films, offering crucial information on the film's suitability for certain uses. Enhancing the efficiency of CdTe-based devices requires optimizing synthesis and characterization procedures.

The structural, optical, electrical, and chemical characteristics of CdTe, CdTe: Zn, and CdS: Mg thin films are largely determined by the synthesis and characterization techniques used. Because of its inexpensive cost, strong absorption coefficient, and advantageous bandgap (about 1.45 eV), CdTe thin films are frequently utilized in solar devices. While characterization techniques are crucial for assessing and improving the films, the synthesis process affects the film's quality, shape, and performance in applications like SCs.

A summary of thin-film deposition methods and a few chosen methods are presented in this chapter, and then the ED method is covered. The computational method and thin film characterization methods are included. These concepts are discussed in the next section.

2.7. Thin Film Deposition Techniques

Various deposition methods have been used to synthesize CdTe, CdZnTe, and CdMgS thin films, such as Close space sublimation (CSS) (Danielson et al., 2023), chemical molecular beam deposition method (CMBD) (Razykov et al., 2017), successive ionic layer adsorption and reaction (SILAR) (Samanta et al., 2017), chemical bath deposition (CBD) (Miya et al., 2022), physical vapor deposition (Yavorskyi et al., 2019), metal-organic chemical vapor deposition (MOCVD) (Oklobia et al., 2022b), pulsed laser deposition (PLD) (Wang et al., 2021), vacuum evaporation (Kumari, Suthar, Himanshu, Kumari, et al., 2022), co-precipitation (Golsefidi et al., 2016), spray pyrolysis (Arce-Plazaa et al., 2017), RF sputtering (Doroody et al., 2021), sol-gel (P. Zhang et al., 2023) and ED (ED) (Olusola et al., 2020). Every deposition strategy has advantages and disadvantages. Among the growth processes mentioned above, CSS and MOCVD make use of

expensive vacuum techniques and highly advanced equipment. It is an abnormal phase transition from a solid to a gas state. Compared to the other approaches, the solution-based approach, like CBD, is less expensive, and the phase transition from liquid to solid state is more organic. However, with this approach, the solutions are thrown away after only one usage. In this instance, less common Te is produced together with a significant amount of hazardous waste, including Cd. However, the ED approach is a superior growth method for CdTe, CdZnTe, and CdMgS thin films compared to the other methods. In particular, the TEED approach is inexpensive and straightforward. We chose this strategy for our investigation. The next part will go into ED, including its kind, benefits, and drawbacks.

2.7.1 ED method

ED is a technique used to deposit a material, typically metal or a metal compound, onto a surface by applying an electric current. This process is commonly used in various fields, including materials science, electroplating, and electronics. Here's a basic overview of how ED works. The process involves an electrolyte solution that contains dissolved metal ions as the precursor for forming a thin film. There are two main electrodes: Anode, the positive electrode, which often consists of the metal to be deposited or a material that facilitates the release of metal ions into the solution. The cathode is the negative electrode, which is the surface on which the metal is deposited. An electrochemical reaction at the anode oxidation occurs, releasing metal ions into the solution. At the Cathode, reduction occurs; metal ions from the solution gain electrons and deposit them onto the surface.

The electroplating circumstances have an impact on the physicochemical properties of CdTe ED layers, and optimizing the deposition variables is one of the most important stages. These factors include the electrodes used, the cathode voltage for deposition, the growth time, the rate of stirring, the temperature at which deposition occurs, the ion concentration in the electrolyte solution, and the pH of the electrolyte solution (Ojo et al., 2021) (Edition et al., 2022). When the material layers are deposited in ED, these six (6) factors must be considered. The details of these parameters are discussed below.

2.7.1.1. Effect of deposition pH

The pH level of the electrolyte solution is one of the primary deposition factors that must be changed to produce high-grade photoconductive film (Yimamu, Afrassa, et al., 2024). In particular, the influence of pH on the growth of CdTe thin film growth will change the composition

and the conductivity of the films. At low pH, Te-rich CdTe thin films were deposited with n-type conductivity, and at higher pH, p-type CdTe, where Cd-rich thin films were deposited. Effect of electrolyte pH during deposition on the unique properties of ED CdTe thin films (Ojo et al., 2021). A major factor in stoichiometric makeup will be pH adjustment. One of the primary concerns throughout ED for the formation of CdTe thin films is hydrogen evolution, which can have a direct effect on the formation of the forming layer (Agasti et al., 2018). This difficulty can be handled by methodically adjusting the pH of an electrolytic solution. The aforementioned study found that the deposition pH significantly influenced the structural, optical, and morphological properties of the thin films.

2.7.1.2. Effect of Ion Concentration and Purity of Precursors

For optimal ED of thin films, it's crucial to carefully control both the ion concentration and the purity of the precursors. Balancing these factors can lead to improved film quality, enhanced performance, and desirable material properties tailored for specific applications. Examining the results of cells made using precursors that range in price and purity might yield important information for device application (A. Alam et al., 2024).

2.7.1.3 Effect of deposition time

The film thickness, which is greatly influenced by the deposition period, determines the layer's absorbance for SC device applications (Yimamu, Afrassa, Dejene, Echendu, Tshabalala, et al., 2023). Under the specified circumstances, it was observed that the structural, optical, morphological, and chemical composition features of the formed CdS films were significantly influenced by the duration of the deposition process. The films became thicker as the deposition time rose. More and more strong CdS XRD peaks appeared as the deposition time increased (Echendu, Mbamara et al., 2016). A detailed investigation has been conducted into the effects of deposition time on the optical, morphological, and structural properties of the CdTe layer formed by ED at different deposition durations (1 h, 2 h, and 3 h). This indicates that crystallinity has improved with deposition time (Verma & Khare, 2024).

2.7.1.4 Effect of deposition voltage

Because altering the deposition voltage allows for the synthesis of *I-n*- and *p*-type CdTe layers, it is the deposition voltage that must be tuned first for the formation of stoichiometric thin films of CdTe. Optimizing the deposition voltage is a little challenging because of the presence of several element ions, including Cd and Te, in the electrolyte solution and the various reduction potentials

(Yimamu, Afrassa, Dejene, Echendu, Terblans, et al., 2023b). The composition of stoichiometric elements in thin-film ED technology is greatly impacted by the adjustment of the deposition voltage (Yimamu, Dejene, et al., 2024).

2.7.1.5 Effect of magnetic stirring

Based on surface morphology and elemental, structural, optical, and electrical characteristics, CdTe layers with favorable optoelectronic properties may be formed on glass/FTO surfaces starting at a solution volume of 100 ml and a stirring rate of between 60 – 85 rpm (Atapattu et al., 2018). It is crucial to create a stirring technique to maintain an ordered flow of solution to the electrode while supplying ions at a pace commensurate with their consumption at its surface (Atapattu et al., 2016). Stirring rate plays a significant role in thin film formation in the ED method.

2.7.1.6. Effect of deposition temperature

The thickness determines the absorber layer, whereas the current density determines the film thickness. While the temperature of the solution, the concentration of Te in the solution, and the glass substrate's cleanliness all affect the current density during deposition, it is still not constant. The ions in the electrolyte bath move more freely, and the solvents become more soluble at higher temperatures. The crystallinity of the film increased along with the deposition rate at increasing current densities. It is crucial to research the impact of deposition temperature (Yimamu et al., n.d.) thoroughly. An analysis was conducted on the impact of deposition temperature on producing high-quality films (Ravichandiran et al., 2018).

2.7.2 Classification of ED

ED, the process of depositing a material from a solution onto a surface using electrical current, can be classified in several ways based on different criteria. Here is a general classification.

2.7.2.1. Based on the electrode utilized

In ED, the electrochemical setup can be classified into TE and three-electrode systems based on the number and type of electrodes used in the process. The main difference between the two is how the current is applied and how the potentials are controlled, which impacts the efficiency and precision of the deposition.

2.7.2.1.1. Three-Electrode Approach

The three-electrode system, the working electrode (the cathode), the counter electrode (the anode), and the reference electrode are used in the conventional ED setup. This system has served as the foundation for the majority of research done on semiconductor ED to date (Echendu, Okeoma, et al., 2016). It is commonly recognized that in a three-electrode system, the reference electrode,

which has a known and steady electrode potential of its own, is used to measure the potential of the working electrode. In commercially available goods, reference electrodes often include an exterior jacket made of saturated KCl solution, which may allow K^+ to seep into the electrolyte (I. M. Dharmadasa, Madugu, et al., 2017b).

2.7.2.1.2. TE Approach

Using a TE setup, ED was done in aqueous solutions in this work. The reference electrode was left out because it may leak and pollute the electrolytes with foreign ions like Ag^+ and K^+ , which would have a negative impact on the SC devices' performance (A. E. Alam et al., 2019).

In this work, CdTe thin films were grown on a conductive glass/FTO substrate using a TE cathodic ED technique in potentiostatic mode. There are a number of benefits to using a TE system, including lowering impurity from the reference electrode in the event of leakage or accidental breakage, saving money because reference electrodes are very costly, and increasing growth rate, allowing them to produce a two μ thickness film in a relatively short amount of time. Additionally, the operating temperature will rise for their potential use in photovoltaics (Journal, 1980).

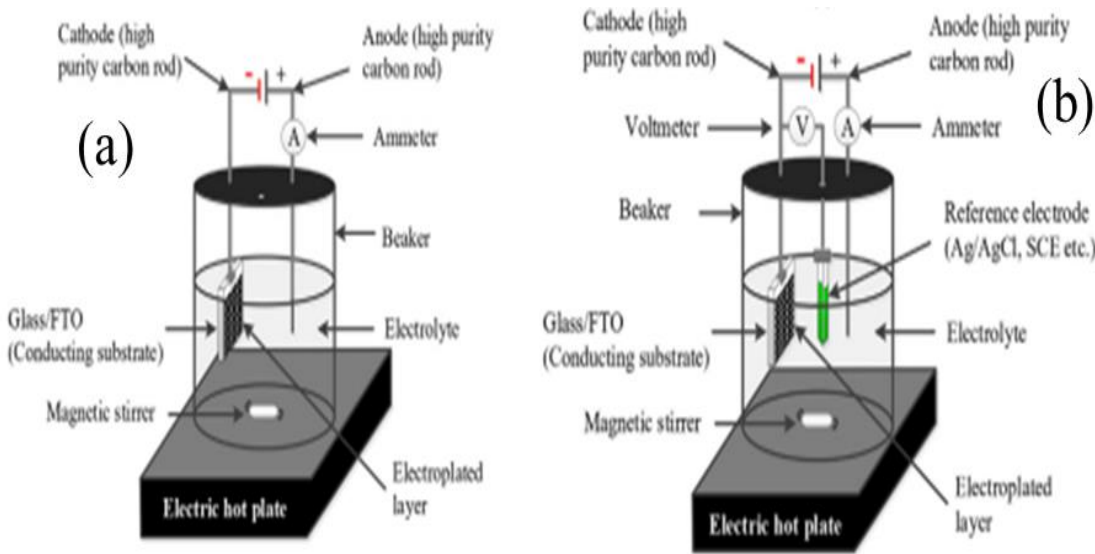


Figure 2. 4.. ED setup (a) TE approach b three-electrode approach (Ali et al., 2021).

In the ED of semiconductors, two electrode systems are typically used for two main reasons: (1) to avoid the possibility of ions like Ag and K contaminating the deposition electrolyte, which can eventually seep into it from the widely used Ag/AgCl and Hg/HgCl (saturated calomel) reference electrodes throughout the ED procedure, particularly when the reference electrode ages; and (2) to

make simpler the ED procedure and thereby lower costs (Echendu, Mbamara, et al., 2016). Because it doesn't require activating agents or surfactants, the ED approach is advantageous for creating scattered metal nanoparticles for electrocatalysts. Instead, controlled electron addition can be employed. As a result, the ED technique produces deposits of pure nanomaterials and is economical. For the galvanostatic ED to produce uniformly sized nanoparticle deposits, the current must remain constant. Generally speaking, the three electrodes used in galvanostatic deposition are the glass carbon working electrode, the platinum coil auxiliary/counter electrode, and Ag/AgCl. The choice of Ag/AgCl and the design of the device are crucial for maximizing absorption and thin-film device performance (Kale et al., 2021). working electrode voltage (potentiostatic mode) or the working electrode current (galvanostatic mode) must be regulated in aqueous deposition (Ali et al., 2021).

2.7.3. The advantage of the ED method

The platform for regulating the material characteristics (optical, structural, morphological, and electrical) by modifying the preparative parameters is another advantage of the ED process [20]. The technology of ED was chosen for semiconductor deposition because, among other benefits, it offered comparative advantages in terms of deposition process continuity, cheap cost, simplicity, scalability, non-vacuum technique, and decrease of waste containing Cd (Ojo & Dharmadasa, 2017). ED is a versatile technique with applications ranging from industrial manufacturing to scientific research, and technological advancements continue to improve its efficiency and precision.

2.7.4. Disadvantage of the ED method

The substrate's conductivity is a crucial prerequisite for the ED process (Olusola et al., 2015). In some cases, post-deposition treatments such as annealing or etching may be necessary to achieve desired film properties, adding additional steps and complexity to the fabrication process. In the case of two-electrode, the current density is not constant, so optimization of deposition conditions is highly required. The deposition needs more purity materials, and most ED methods are in aqueous solution. The boiling point of water is 100 C, so it is limited to deposited at low temperatures.

2.8. Density Functional Theory (DFT)

The Schrodinger equation covers every issue pertaining to the electronic structure of matter, including the quantity of electrons and the location of nuclei. Thus, we concentrate on the Schrödinger equation that is independent of time. The Schrödinger equation describes a system of

particles through a wavefunction, which depends on the positions of all particles in the system. For a system with N particles (such as electrons in an atom or molecules), the wavefunction depends on 3N spatial coordinates (in three dimensions), leading to an exponential increase in the number of variables as the number of particles grows. In this case, a more complete description of the Schrodinger is

$$\left[\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + \sum_{i=1}^N V(ri) + \sum_{i=1}^N \sum_{j < i} U(ri, rj) \right] \varphi = \epsilon \varphi \quad 2.1$$

Where m stands for electron mass in this case. This equation's three bracketed variables denote, in order, the kinetic energy of each individual electron, the interacting energy between each individual electron and the group of atomic nuclei, and the interacting energy between various electrons.

Although the electron wave function is a function of each of the coordinates of all N electrons, is possible to approximate φ as a product of individual electron wave functions, $\varphi = \varphi_1(r)\varphi_2(r)\varphi_3(r) \dots \varphi_N(r)$. This expression for the wave function is known as a Hartree product. While the Schrödinger equation is a foundational tool in quantum mechanics, its limitations in dealing with many-body interactions, large systems, and electron correlation have led to the development of approximate methods like DFT and Hartree-Fock theory. These methods simplify the problem, often by reducing the complexity of the wavefunction or focusing on quantities like electron density instead of the full wavefunction. Despite these limitations, the Schrödinger equation remains central to understanding quantum systems. Different approximations were applied to the nature of the electron and its surroundings to solve this. Numerous electrons interacting with numerous nuclei is a more complex scenario that interests us. A more thorough explanation of the Schrodinger in this instance.

2.8.1. Born-Oppenheimer Approximation

The Born-Oppenheimer approximation is crucial for calculations involving electronic structures. One of the most important discoveries when applying quantum mechanics to atoms is that atomic nuclei are significantly heavier than individual electrons; each proton or neutron in a nucleus has more than 1800 times the mass of an electron. This indicates that electrons react to environmental changes far more quickly than nuclei. This allows us to divide our physical inquiry into two parts. The equations describing the travel of electrons are first solved for fixed locations of the atomic nuclei. We identify the state, or smallest-energy configuration, of a particular set of electrons flowing in a set of nuclei's field. The electrons' ground state is their lowest energy state, and

separating the nuclei and Born-Oppenheimer approximation is the process of splitting electrons into discrete mathematical issues.

2.8.2 . Hartree- Fock approximation

In the Hartree-Fock approximation, the system's total wavefunction is a product of individual electron wavefunctions, but the individual wavefunctions are determined by solving the self-consistent Hartree-Fock equations. These equations are derived by minimizing the energy function subject to the constraint that the total wave function must remain antisymmetric. However, while the Hartree-Fock approach accounts for exchange effects (due to the antisymmetric of the wavefunction), it still ignores electron correlation effects, which are crucial for more accurate treatments of many electron systems.

he Hartree product refers to an approximation for the total wavefunction of a many-electron system in which the total wavefunction is assumed to be a product of single-particle wavefunctions.

For a system of N electrons, the total wavefunction $\varphi(r_1, r_2, r_3 \dots r_N)$ is a function that describes the quantum state of all N electrons in the system. In principle, this wavefunction should account for the correlations between all the particles, including exchange effects and electron-electron correlations. However, exact solutions to the many-body Schrödinger equation are often difficult or impossible to obtain, especially for systems with many particles. The Hartree product provides a simplification by assuming that the total wavefunction is separable into individual wavefunctions for each electron, which ignores electron-electron correlations. The Hartree product is mathematically expressed as:

$$\varphi(r_1, r_2, r_3 \dots r_N) = \varphi_1(r_1)\varphi_2(r_2)\varphi_3(r_3) \dots \dots \dots \varphi_N(r_N) \quad 2.2$$

Here, each $\varphi_i(r_i)$ is the single-particle wavefunction for the i-th electron.

Density Functional Theory has evolved from a theoretical framework to a powerful computational tool, making it one of the most important methods in quantum chemistry, material science, and condensed matter physics. Its development, from the foundational Hohenberg-Kohn and Kohn-Sham theorems to modern functionals, has drastically improved our ability to understand and predict the properties of complex systems. Despite its challenges, DFT continues to grow in accuracy and applicability, remaining central to computational investigations of the electronic structure. Two fundamental mathematical theorems established by Kohn and Hohenberg form the foundation of the whole area of density functional theory.

The first theorem, proved by Hohenberg and Kohn, is that the ground-state energy from Schrodinger's equation is a unique function of the electron density. Another way to restate According to the findings of Hohenberg and Kohn, the ground-state electron density is the only factor that can define all of the ground state's characteristics, including its energy and wave function.

The second Hohenberg–Kohn theorem defines an essential property of the function: The electron density that minimizes the energy of the overall function is the true electron density corresponding to the complete solution of the Schrodinger equation. These theorems establish the groundwork for DFT, suggesting that all the properties of a system can be determined if the electron density is known rather than requiring the full many-body wave function.

2.8.3 Kohn-Sham Equations

While the Hohenberg-Kohn theorems establish the fundamental principles of DFT, the practical application of DFT was made possible by the Kohn-Sham equations (1965), developed by W. Kohn and L.J. Sham. The idea behind the Kohn-Sham approach is to replace the interacting many-electron system with a fictitious system of non-interacting electrons that produce the same electron density. The Kohn–Sham equations have the form

$$\left[\frac{\hbar^2}{2m} \nabla^2 + V(r) + V_H(r) + V_{XC}(r) \right] \varphi_i(r) = \epsilon_i \varphi_i(r) \quad 2.3$$

Kohn–Sham equations there are three potentials $V(r) + V_H(r) + V_{XC}(r)$ are potential defines the interaction between an electron and the collection of atomic nuclei. The second is called the Hartree potential and is defined by

$$V_H(r) = e^2 \int \frac{n(r') d^3 r'}{|r - r'|} \quad 2.4$$

$V_{XC}(r)$ which defines exchange and correlation- contributions to the single electron equations. It can formally be defined as a functional derivative of the exchange-correlation energy. The Kohn-Sham equations describe a system of non-interacting particles moving in an effective potential, which includes contributions from the external potential (like the nuclei) and the electron-electron interactions. The Kohn-Sham approach allows one to solve the problem of interacting electrons by solving a set of single-particle Schrödinger equations for non-interacting electrons, but with an effective potential that accounts for the interactions.

2.8.4. Exchange-Correlation Functional

One of the main challenges in DFT is dealing with the exchange-correlation function, which describes the effects of electron exchange (the Pauli exclusion principle) and correlation (the dynamic interaction between electrons) beyond the classical Coulomb interaction. The exact form of the exchange-correlation function is not known, and as a result, approximations are made to simplify the calculations. Two of the most commonly used approximations are:

2.8.4.1. Local Density Approximation (LDA)

Assumes that the exchange-correlation energy at any point in space depends only on the local electron density at that point. This approximation works well for systems where the electron density is nearly uniform.

2.8.4.2. Generalized Gradient Approximation (GGA):

Extends LDA by including the gradient of the electron density, providing a more accurate description of the exchange-correlation energy, especially for inhomogeneous systems like molecules and surfaces.

2.8.5 Steps in a Typical DFT Calculation

1. Initial Guess: Start with an initial guess for the electron density $\rho(r)$
2. Solve Kohn-Sham Equations: Using the initial density, solve the Kohn-Sham equations to find the one-particle wavefunctions and eigenvalues. This gives the electron density $\rho(r)$ from the wavefunctions.
3. Update the Electron Density the acquired wavefunctions are used to update the electron density.
4. Repeat: Iterate this process of solving the Kohn-Sham equations and updating the density until self-consistency is reached, meaning the density no longer changes significantly between iterations.

5. Calculate Properties: Once the self-consistent electron density is obtained, the total energy and other properties (such as the molecular geometry, bond strengths, etc.) can be computed.

According to the DFT formalism, one may use the electron density distribution $n(r)$ alone to derive the ground state (GS) and additional features of an electron arrangement in a field outside of it (Jones, 2015). Using DFT, one may describe the ground state characteristics of insulators, semiconductors, and metals. It is possible to use this theory to determine a many-electron system by employing functional functions or functions of another function, in this instance, the spatially dependent electron density. It gives you a way to find the cut-off energy, total energy, total minimum energy, k-points, and crystal structural characteristics.

The Quantum ESPRESSO, an acronym for opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization suite, which is freely available as free software under the GNU General Public License, is used for first-principles electronic structure computations and materials modeling. DFT, plane wave basis sets, and pseudopotentials (both ultra-soft and norm-conserving) form their foundation.

One of the challenges in thin film CdTe for SE application is the toxicity of Cd for synthesis and the lower abundance of Te because it is a rare earth metal. The best method for this costly and safety problem is the computational method. DFT has become the most popular and low-cost method of electronic structure calculation, with good agreement for experimental value in computational physics. The electron structure aspects of materials were critical in improving their applicability for SCs and other device applications (Othman et al., 2012).

In density functional theory, the many-electron wave function problem is replaced by electron density. It is a computational method for the approximate solution of the Schrodinger equation. It was founded on the concept that electrons in the materials behaved similarly to those in a homogeneous gas, and the influence of the non-valence electron and the nucleus (the frozen core) was modeled using a pseudo-potential approach. The computation considered just the outermost electrons of each atom (Bahloul et al., 2015). Quantum mechanics density functional theory is frequently used to make precise computations on atomic, molecule, and condensed matter systems. First-principles DFT), the LDA, and the GGA were used to calculate total energy, structure, and band structure properties (Ma et al., 2020). The optical parameters examined as a function of photon energy include the real and imaginary components of the dielectric function, the absorption coefficient, and the energy loss function (Edossa & Woldemariam, 2020). Hybrid density functional approximation is excellent in properly representing the material's properties, especially band gap calculation (Heyd et al., 2003).

3. Materials and Method

3. 1. Materials

3.1.1 Chemicals, Solvents and Equipment

The chemical precursor's salts for ED of CdTe, CdTe: Zn, and CdS: Mg thin films were cadmium acetate dihydrate [$\text{Cd}(\text{CH}_3\text{OO})_2 \cdot 2\text{H}_2\text{O}$] with 98% purity, Cadmium chloride (CdCl_2) as cadmium precursor, zinc acetate dihydrate [$\text{Zn}(\text{CH}_3\text{CO}_2)_2 \cdot 2\text{H}_2\text{O}$], with 98% purity as a Zn precursor, magnesium chloride (MgCl_2) as Mg dopant source were used. The other chemicals are tellurium dioxide (TeO_2), with 98% purity as a tellurium precursor, and sodium thiosulphate ($\text{Na}_2\text{S}_2\text{O}_3$) as S precursors. Diluted hydrochloric acid (HCl) and ammonium hydroxide (NH_4OH) are used to arrange the pH. The conductive glass/fluorine-doped tin oxide (FTO) substrate deposits films. Deionized water (DI) was used to prepare the solution and clean the glass substrate. Solvents such as ethanol, acetone, and methanol were used to clean the glass FTO substrate. Gill AC potentiostatic, computer, and glass bikers are used for EDs of thin films.

3.2 Method

3.2.1 Experimental method

CdTe thin films were grown from an electrolyte solution containing 1.0 M of cadmium acetate dihydrate [$\text{Cd}(\text{CH}_3\text{OO})_2 \cdot 2\text{H}_2\text{O}$] with 98% purity as cadmium precursor and 2 ml of tellurium dioxide TeO_2 with 99% purity as tellurium precursor by electrochemical deposition method. Both chemicals were laboratory reagent grade with $\text{Cd}(\text{CH}_3\text{OO})_2 \cdot 2\text{H}_2\text{O}$ and TeO_2 were purchased from Sigma Aldrich.

On a coated glass/FTO substrate with a sheet resistance of 8 ohm/square, these thin films were applied using the TEED technique. The glass substrate was cut into 2.5×2.5 cm pieces, ultrasonically cleaned, and then dried in air after being treated with ethanol, acetone, and methanol, respectively. At room temperature, the electrolyte solution's pH was kept at 2.00. The electrolyte solution bath's deposition temperature was kept at 85 °C, and the magnetic stirrer agitated the solution reasonably during the deposition process. A Gill AC potentiostatic computer was utilized as the electrical power supply for the two electrodes (ACM instrument, United Kingdom). The glass substrate was affixed to the carbon plate, which served as the cathode (working electrode), and the graphite rod as the anode (counter electrode) using insulating polytetrafluoroethylene (PTFE) thread seal tape

Cd-containing solution having 1 M $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ was prepared in 400 ml deionized (DI) water in a 600 ml beaker and stirred for 1 hour. The Te-containing solution was prepared by dissolving 2g of TeO_2 in 30 ml of dilute HCl in a 50 ml beaker and then stirred for 2 hours since Te is a semi-metallic element that is soluble in an acidic medium. From the solution, only 2 ml of Te-containing solution was added to the Cd-contained solution and then stirred for 5 hours to keep the uniformity of the solution, and the deposition was done without further purification. Measurements using cyclic voltammetry (CV) were made in order to maximize the deposition voltage range. CdTe was deposited in the voltage range of (1200-1450) mV based on the study of CV measurements. The voltage range in which the deposition took place was 50 mV intervals (1200, 1250, 1300, 1350, 1400, and 1450 mV). The film was grown for two hours while all other parameters remained the same. For each sample, the ED CdTe thin film's optical, electrical, and structural characteristics were examined.

The electrolytic method used for producing CdTe thin films involved the preparation of a solution containing cadmium acetate dihydrate and tellurium dioxide as the precursors. The cadmium precursor consisted of 1.0 M $[\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}]$ with a purity of 98%, purchased from Sigma-Aldrich. The tellurium precursor was 1 ml of (TeO_2) with 98% purity, also obtained from Sigma-Aldrich.

In the first step, a 600 ml beaker was used to prepare the cadmium solution. To this, 400 ml of deionized water was mixed with the 1.0 M cadmium acetate dihydrate. Since tellurium (Te) is known to be soluble and stable in acidic media, a separate solution was prepared by dissolving 2 g of TeO_2 in 30 ml of diluted hydrochloric acid (HCl). This mixture was stirred for two hours to ensure complete dissolution of the TeO_2 . After this, 1 ml of the tellurium-containing solution was added to the cadmium acetate solution in the 600 ml beaker.

The deposition process was carried out under controlled conditions, with the temperature maintained at 85°C, a deposition voltage of 1250 mV, and a deposition time of 120 minutes. The films were deposited under different pH values of the electrochemical solution, specifically pH values of 1.8, 2.5, 3.0, and 3.5. To adjust the pH of the solution, ammonium hydroxide (NH_4OH) or diluted hydrochloric acid (HCl) was used. The electrolyte solution was continuously agitated during the deposition using a magnetic stirrer at a moderate stirring rate to ensure uniform mixing. By keeping the deposition parameters constant and adjusting the pH of the solution, the effects of different pH values on the deposition of CdTe thin films were studied.

After preparation, each sample was divided into two halves. One half was left in its as-prepared state, while the other half was immersed in a CdCl_2 solution for 1 minute, with the pH of the solution adjusted to 3.0. Following immersion, the samples were air-dried and then annealed at 400°C for 20 minutes. Prior to the deposition of the CdTe thin films, the cadmium acetate solution was electro-cleaned for 48 hours at a voltage lower than that of elemental Cd, as determined by cyclic voltammetry. This cleaning process was necessary to remove metallic ion contaminants from the electrolyte, as the Cd source used in this study was not highly pure. For CdTe thin film deposition, the FTO was connected to the working electrode, washed with deionized water, and then submerged in the electrolytic solution for 120 minutes. The cathode voltage was set to 1250 mV, and the pH values of the deposition solution were adjusted to 1.8, 2.5, 3.0, and 3.5, with moderate agitation during the process. After deposition, the samples were removed from the solution, cleaned with deionized water, and allowed to air dry. The ideal deposition pH for the formation of CdTe thin films in a TE potentiostatic configuration was determined by analyzing the samples' structural, optical, electrical, surface morphology, elemental composition, and surface roughness characteristics. Both the as-deposited and heat-treated thin films were examined for their structural, optical, conductivity, surface morphology, composition, and surface roughness properties.

For the ED of CdZnTe thin films, the electrolyte solution consisted of 1.0 M cadmium acetate dihydrate $[\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}]$, with 98% purity, as the cadmium precursor, along with varying concentrations of zinc acetate dihydrate $[\text{Zn}(\text{CH}_3\text{CO}_2)_2 \cdot 2\text{H}_2\text{O}]$, also with 98% purity, at concentrations of 0.25, 0.50, 0.75, and 1.00 M as the zinc precursor. Additionally, 1 ml of 99% pure tellurium dioxide (TeO_2) was included as the tellurium precursor.

The thin films were deposited using a TEED method onto glass substrates coated FTO, which had a sheet resistance of 8 ohms per square. The glass/FTO substrates, each measuring $2.5\text{ cm} \times 2.5\text{ cm}$, were first cut to size before ED (ED). They were then ultrasonically cleaned for 30 minutes using a laboratory soap solution mixed with deionized water. After this, the substrates were sequentially cleaned with ethanol, acetone, and methanol. Finally, the substrates were rinsed with deionized water and left to air dry.

To adjust the pH of the electrolyte solution to 3.00, either ammonium hydroxide (NH_4OH) or diluted hydrochloric acid (HCl) was used. The electrolyte bath was maintained at a temperature of

85°C during the deposition process. The concentration of zinc in the solution was varied at four different levels (0.25, 0.50, 0.75, and 1.00 M), while the deposition voltage was kept constant at 1750 mV. A magnetic stirrer was used to agitate the solution at a moderate speed to ensure uniformity throughout the deposition process.

The Cd and Te precursors were added to the deionized water of 400 ml, the solution was stirred, and the Zn precursor was added. On the other hand, the Te-containing solution was created by dissolving 2 gm of TeO_2 in 30 ml of diluted HCl solution and stirring for 20 minutes. Te is soluble in an acidic environment but insoluble in water. To maintain the homogeneity of the Cd and Zn-containing solution, 1 ml of Te-containing solution was added, and the mixture was then stirred for 5 hours.

The conductive glass substrate that was previously cleaned and affixed to the working electrode was once again cleaned with deionized water and submerged in the electrolyte solution for a duration of 120 minutes in order to deposit CdZnTe thin films for 0.25 M Zn concentration. After being taken out of the solution, cleaned with deionized water, and the sample was dried in the air. The steps continued for 0.50, 0.75, and 1.00 M Zn concentration.

For the ED of CdS:Mg thin films, cadmium chloride (CdCl_2) was used as the cadmium precursor, magnesium chloride (MgCl_2) as the magnesium dopant source, and sodium thiosulfate ($\text{Na}_2\text{S}_2\text{O}_3$) as the sulfur (S) source. All chemicals were of laboratory reagent grade, purchased from Emsure Germany, with a purity of 99.0%. ITO substrates were employed for the thin film deposition. The electrolyte solution for growing CdS:Mg thin films was prepared by dissolving 0.3 M cadmium chloride (CdCl_2), 0.06 M magnesium chloride (MgCl_2), and 0.03 M sodium thiosulfate ($\text{Na}_2\text{S}_2\text{O}_3$) in 400 mL of deionized water. To maintain the pH of the electrolytic solution at 1.8 ± 0.02 , diluted hydrochloric acid (HCl) and ammonium hydroxide (NH_4OH) were used for pH adjustment. The deposition process was carried out at a temperature of 85°C for a duration of 30 minutes.

To optimize the growth of CdS:Mg thin films, the cathodic deposition voltage was carefully adjusted. The deposition was conducted using a TEsetup powered by a Gill AC potentiostat (ACM Instrument, United Kingdom), which was computer-controlled for precise voltage regulation. In this setup, the working electrode (cathode) was the glass/ITO substrate, which was connected to a graphite rod using PTFE thread seal tape. The counter electrode, or anode, was another graphite rod. This configuration allowed for efficient deposition of CdS:Mg thin films.

3.2.2. Computational Method

Geometry, structural optimization, and ground state energy calculations have been done using the plane wave self-consistence field (PWSCF) base set method within the DFT as implemented in the quantum espresso package. One of the challenges in DFT is that exchange-correlation functional can be approximated using the LDA, and GGA depends on the gradient of the local density is the Perdew–Burke-Ernzerh of functional (PBE). For band gap calculations, we used the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional in addition to LDA to get the real energy band gap of the materials, and for better computational output, the energy difference convergence test is performed in k _ point mesh, lattice parameter calculation, and kinetic energy cutoff which is less than 0.1 meV. For this calculation, we use the integrated reciprocal for the first Brillouin zone, the k _ point mesh 6x6x6 Monkhorst-Pack grids, and the kinetic energy cutoff PWSCF calculation the plane-wave expansion of the basic functions was set 70 Ry for LDA and GGA all the structure optimizations, the force and energy convergence considered.

To reduce the computational exchange-correlation approximation error, we perform the convergence test for k -point mesh and total energy and kinetic energy cutoff as a function of total energy convergence (Ry).

3.2.3. Characterizations Method

The ED thin films were characterized by using X-ray diffraction (XRD), scanning electron microscopy (SEM), scanning probe microscopy (SPM), Photoelectrochemical cell study, UV–VIS spectrophotometry, Raman spectroscopy (RS), energy-dispersive X-ray spectroscopy (EDS) to study the structural, surface morphology, surface roughness, electrical, optical and compositional properties were done for optimization of deposition parameters the most important tasks in producing high-quality CdTe thin films for the intended use is optimizing the deposition parameters. Deposition voltage, growth time, pH of the solution, rate of stirring, temperature of deposition, ion concentration in the electrolyte solution, and electrodes utilized are some of these characteristics. The most important of these factors to first adjust for the creation of stoichiometric thin films of CdTe formations is the deposition voltage.

Additionally, the following formulae are used to derive the structural characteristics. When the incident rays come into contact with the sample, Bragg's law indicates that constructive interference (as well as a diffracted ray) is produced.

$$n\lambda = 2d\sin\theta \quad 3.1$$

Where n is an integer, d is the interplanar distance that causes the diffraction, θ is the diffraction angle, and λ is the wavelength of the X-rays.

The crystallite size, D , of the ED CdTe thin film, was calculated using Scherer's formula in equation 3.2 (Mahato et al., 2015)

$$D = \frac{0.9 \lambda}{\beta \cos \theta} \quad 3.2$$

where β is the full width at half maximum (FWHM) in radian, λ is the wavelength of the X-rays (0.15406 nm for Cu K α), and θ is the Bragg's diffraction angle in degree.

The dislocation density, which describes the length of dislocation lines per unit volume of the crystal in the CdTe thin-film via ED technique, is estimated using equations provided in the literature (3.3) (Ozmen & Gubur, 2022)

$$\delta = \frac{1}{D^2} \quad 3.3$$

Where δ dislocation density and D is crystallite size

The microstrain (ϵ) can be calculated by using the relation in equation (3.4) (Amin et al., 2022)

$$\epsilon = \frac{\beta_{hkl}}{4 \tan \theta} \quad 3.4$$

4. Results and discussion

4.1. Optimization deposition voltage for CdTe

4.1.1. Cyclic Voltammetry Study (CV)

In thin film deposition techniques, Cathode Voltage (V_g) controls the energy of the electrons and the ions in the system, which in turn influences the growth rate and the properties of the film. The voltage can affect the film thickness, crystallinity, and other important film properties.

Cyclic Voltammetry is a useful study that aids in the ED of CdTe, providing insights into the electrochemical behavior, deposition kinetics, and mechanism of CdTe film formation. Researchers can optimize conditions for high-quality CdTe deposition for applications in SCs and other electronic devices by analyzing the CV curves. The CV measurements were performed on the electrolyte solutions containing 1.0 M Cd $(\text{CH}_3\text{OO})_2 \cdot 2\text{H}_2\text{O}$ and 2 ml of TeO_2 in 400 ml of DI water. During CV measurements, the deposition temperature was maintained at 85° C. Temperature plays a crucial role in electrochemical reactions and can influence several factors, such as reaction kinetics, electrolyte properties, and the size and uniformity of the deposited particles or films. The electrolytic solution pH was adjusted to 2.00. The acidic environment influences the electrochemical behavior of the deposited material, such as ion availability, dissolution, and electrolyte stability. The cathodic deposition voltage range of 0–2000 mV implies that the voltage applied to the working electrode is gradually increased from 0 V (no applied voltage) to 2 V. This voltage sweep controls the rate and extent of material deposition and is applied during the cyclic voltammetry with the cyclic sweep of 10mV/s, as shown in Figure 4.1. For the ED of CdTe thin films, optimizing deposition parameters is significant for the growth of the stoichiometric composition of both elements in the thin film. Growth voltage optimization is the first task in the film deposition. CV were used to investigate the range of growth of CdTe thin films. Tellurium deposits first during the ED process because its standard reduction potential is +593 mV concerning the typical H_2 electrode, which is more favorable than that of cadmium with a standard reduction potential value of –403 mV (Ojo & Dharmadasa, 2017).

Figure 4.1 shows that in the forward direction, Te began to deposit at a cathode voltage of 290 mV near region (A). As the voltage is increased to 945 mV near region (B), Cd starts to deposit. In these regions, co-deposition of Cd and Te appeared on the substrate, and the thin film was Te-rich. The current density was in the range of CdTe thin film deposition when the voltage increased from (1200 -1450) mV near region (C). Further increase in cathode voltage (1450-1500) mV near region

(D), Cd-rich CdTe thin films were formed. Beyond 1500 mV, there is a high increase in current density, which is hydrogen evolution at the cathode or Cd dendrites formation, and these were also observed and reported by Diso et al (Diso et al., 2016).

In the reverse direction of the CV measurement, as illustrated in Figure 4.2, a negative current density was detected, indicating the removal of elemental Cd, CdTe, and Te from the cathode surface. This demonstrates that CV measurements are essential for optimizing the voltage range used during deposition.

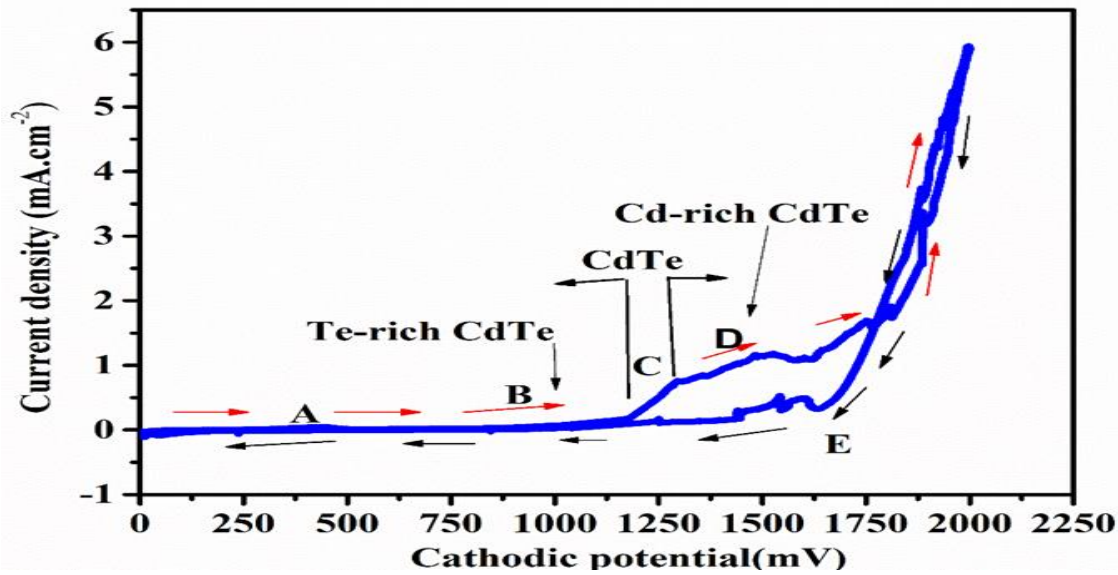


Figure 4. 1. A typical CV measurement for two electrode-electrolyte solutions containing 1.0 M Cd (CH₃OO)₂.2H₂O and 2 ml of TeO₂.

4.1.2. Structural properties of CdTe thin films

The D8 Advance diffractometer is a high-quality instrument used for X-ray diffraction analysis. It typically uses a monochromatic X-ray source, a goniometer for precise angle measurements, and detectors to collect the diffracted X-rays. The D8 Advance system is designed to handle a wide range of samples, making it suitable for characterizing thin films like the CdTe layers grown on glass/FTO substrates. The X-ray generator tension and current were kept at 40 kV and 40 mA, respectively. The XRD measurements were performed in a 2θ range from 20 to 70°.

The structural parameters such as crystallite size, dislocation density, microstrain, and crystallite size per unit area were calculated by utilizing equation (3.1-3.5).

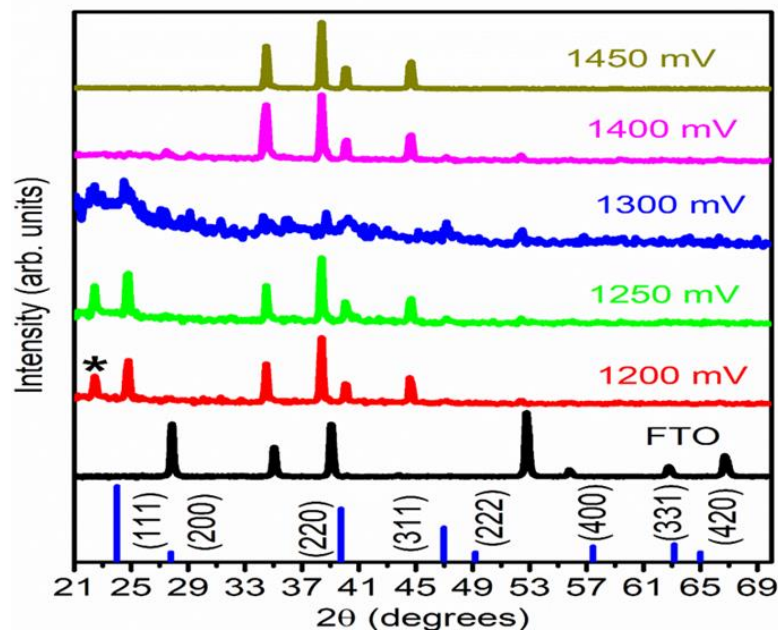


Figure 4. 2. XRD spectra of CdTe thin films with different deposition voltage

Figure 4.2 indicates the polycrystalline cubic zinc mix architectures of CdTe thin films, and the preferential (111) peak intensity varies with deposition voltage. At the voltage of 1200 mV, a peak at 22.9° is attributed to Cd_xTeO_y (Salim, Patel, et al., 2015), which shows that a Te-rich CdTe thin film was deposited, and the crystallite size was 20 nm with an FWHM of 0.40. At a voltage of 1250 mV, several significant changes are observed in the CdTe thin film's X-ray diffraction (XRD) pattern. The intensity of the tellurium (Te) peak is reduced. This indicates that as the voltage increases to 1250 mV, the amount of elemental tellurium in the film decreases, likely due to the more efficient incorporation of cadmium (Cd) into the crystal lattice, leading to a purer CdTe (cadmium telluride) phase. Te peaks in the XRD pattern suggest that elemental Te might be present as a separate phase in the film. The reduction in the Te peak at 1250 mV suggests a shift toward a more stoichiometric CdTe phase with fewer unincorporated Te atoms.

The diffraction peak associated with the (111) plane becomes more intense. This suggests that the CdTe thin film exhibits a preferential (111) orientation, meaning that the crystal grains align more favorably along this direction. The (111) plane is often preferred in the deposition of CdTe thin films because it is energetically favorable and generally associated with better electrical and optical properties in photovoltaic devices. The preferential orientation enhances the material's

crystallinity and can lead to improved charge transport and light absorption in applications such as SCs.

Improved crystallinity, the reduction in the Te peak, and the increase in (111) peak intensity together indicate an enhancement of the CdTe film's crystal structure. The material becomes more ordered at 1250 mV, with fewer amorphous regions and defects, which is critical for the performance of semiconductor devices.

The estimated crystallite size was 26 nm, while the FWHM was reduced to 0.31. For 1400 mV voltage, the FWHM was increased to 0.92, and the crystallite size was compacted to 9 nm. When the voltage was further increased to 1450 mV, the CdTe thin film showed amorphous nature. From the results observed in our study, it is clear that the deposition voltage has a significant impact on the crystallite size of ED CdTe thin films. Lower deposition voltages favor Te-rich CdTe with smaller crystallite sizes. Higher deposition voltages rise the nucleation rate and diminish the crystallite size, which can lead to more defects and lower material quality.

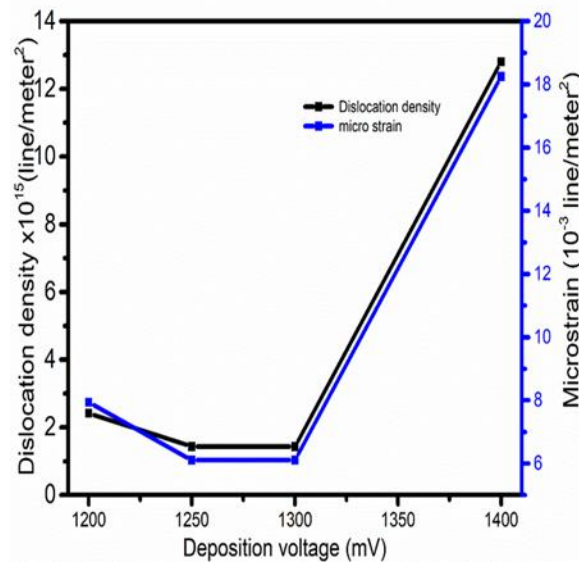


Figure 4. 3. Dislocation density and microstrain vs deposition voltage.

Excessively high voltages may lead to a loss of crystallinity, even causing the material to become amorphous, which would make it unsuitable for many high-performance applications. Therefore, controlling the deposition voltage is crucial for tailoring the crystallite size and optimizing the properties of CdTe thin films for specific applications, especially in devices like photovoltaic cells, where crystallinity has a significant impact on selecting the performance. The results agree with the JCPDS card of 752083 and other published reports (Echendu, Okeoma, et al., 2016).

Figure 4.3 shows that the dislocation density at 1200 mV deposition voltage is 2.4×10^{15} line /meter². When the deposition voltage is 1250, the dislocation density is 1.4×10^{15} line /meter². With an extra voltage bump to 1400 mV, the dislocation density was increased to 12.8×10^{15} line /meter². Figure 4.3 also confirmed that the microstrain at a deposition voltage of 1200 mV is 7.9×10^{-3} line/meter². The decrement in microstrain was visible when the deposition voltage was increased to 1250 mV, and it was recorded as 6.10×10^{-3} line/meter². Further increase in deposition voltage to 1400 mV, the microstrain was increased to 18.25×10^{-3} line/meter². From these two analyses, low dislocation density and microstrain were observed. Further optimization in the range between 1250 to 1300 mV was done, but this is not reported in this paper.

4.1.3. Optical properties of CdTe thin films

Optical absorbance properties were investigated by using UV- VIS spectrophotometry wins lab-scan lambda 950. The absorbance as a function of wavelength was demonstrated in Figure 4.4 (a). The minimum absorbance was recorded at 1450 mV due to Cd-rich, thin films, and the maximum absorbance was at 1250 mV, showing better Cd and Te composition. High absorbance is required for CdTe thin film for the absorber layer in SC applications. Therefore, 1250 mV was the best deposition voltage, this agrees well with the XRD findings.

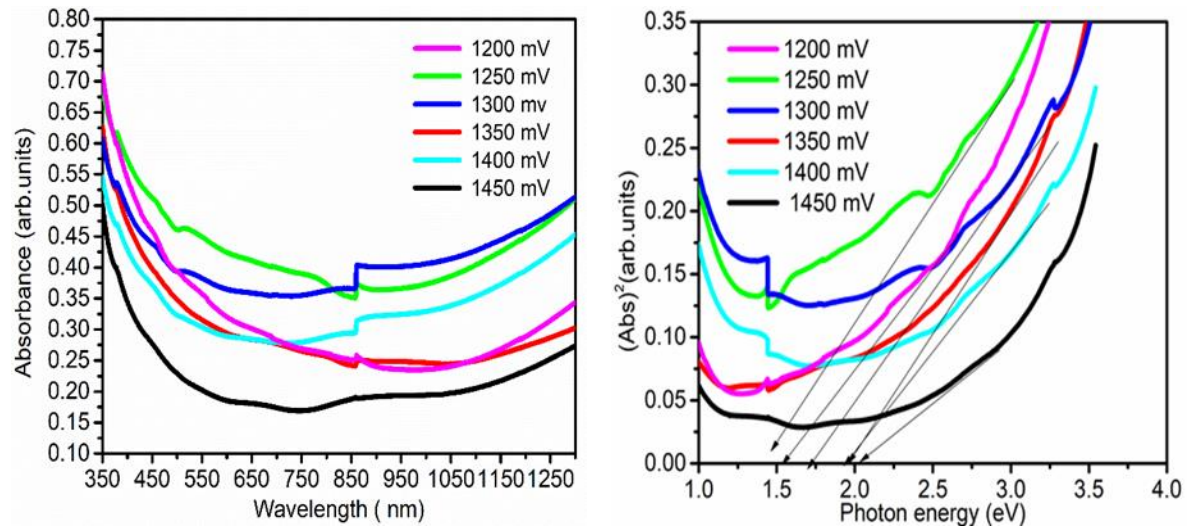


Figure 4. 4 (a) the absorbance vs wavelength (nm) (b) (absorbance)² vs photon energy (eV)

As shown in Figure 4.4 (b), Plotting the absorbance square against photon energy with axis ((abs)² = 0). and extrapolating a tangent line to the graph in order to get the optical energy band gap The energy band gap of ED CdTe varies as deposition voltage varies. Accordingly, at deposition voltages of 1200, 1250, 1300, 1350, 1400, and 1450 mV, the energy band gap was recorded at 1.55,

1.46, 1.71, 1.95, 1.95, and 2.02 eV, respectively. From the experimental analysis, the energy band gap of the ED CdTe thin film deposited at 1250 mV is 1.46 eV, approximately near the bulk energy band gap of CdTe of 1.45 eV (Kuddus et al., 2021).

4.1.4. Photoelectrochemical cell study

The electrical conductivity types of ED-CdTe layers were estimated using photoelectrochemical cell (PEC) studies.

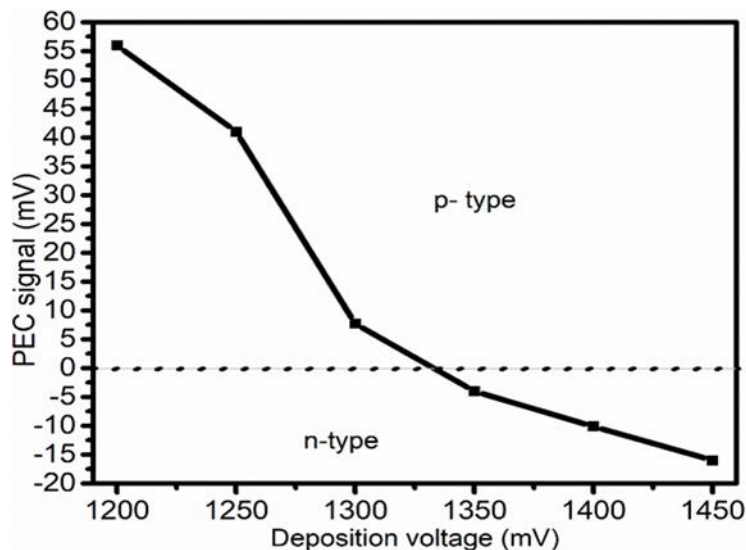


Figure 4. 5. PEC measurements for different deposition voltage

By immersing graphite rod as the anode and glass, FTO, or CdTe as the cathode, this experimental method was used to investigate the potential barrier creation at the solid/liquid interface between CdTe and an appropriate electrolyte solution. The anode was connected to a digital voltmeter, which measured the potential when the circuit was illuminated and in darkness (Ojo et al., 2021). The PEC results were the difference between the voltages under illumination and the dark. The electrolyte solution containing 0.1 M Na_2SO_4 in 20 ml of deionized water in a 50 ml beaker was stirred for 2 hours to make it uniform. Figure 4.5 shows that the conductivity of CdTe thin film at deposition voltage of 1200 to 1350 mV is p-type, while at 1350 to 1450 mV, it becomes n-type. This is due to the excess of Te and Cd in the film. In addition, the material's conductivity was changing due to the presence of Cl in the film. The results agree with the other Cd sources for CdTe thin film (A. A. O. I. M. Dharmadasa, 2017).

4.2. Optimization of pH for CdTe thin films

4.2.1. Structural properties

The electrolytic pH of the deposition solution can dramatically alter the phase formation and crystallinity of the CdTe thin films. The pH influences the reduction potential of the Cd and Te ions, the nucleation density, and the growth rate of the crystals during ED. To assess the effects of heat treatment, XRD is performed both on the as-deposited films (directly after ED) and on films that have undergone heat treatment (annealing)

The XRD spectra of CdTe thin film samples as-deposited and after heat treatment are displayed in Figure 4.6 (a) and (b). The analysis demonstrated that the ED CdTe thin films include hexagonal and cubic zinc mix structures. At 24.04° , the 2θ value is where the (111) favored orientation is located. The higher the deposition pH, the greater its peak intensity. According to the planes of (200), (220), (311), (400), and (331), respectively, the additional peaks are also seen at 27.91° , 40.09° , 47.02° , 57.25° , and 63.42° . With diffraction planes of (110), (111), and (107), the hexagonal phase is seen at 2θ angles of 41.2° , 43.3° , and 68.8° , respectively, for both AD and HT samples with different pH.

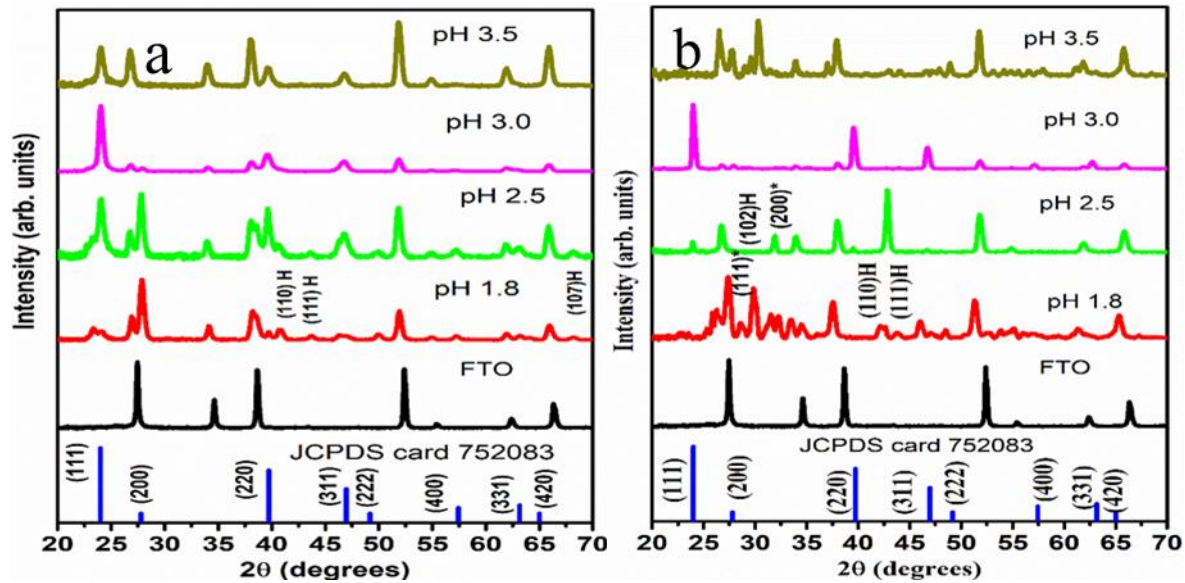


Figure 4. 6 CdTe thin-film XRD patterns grown at different pH values (a) AD and (b) HT

Both the AD and HT samples showed both cubic and hexagonal configurations when the films were deposited at pH values of 1.8 and 2.5. One observes a single-phase cubic CdTe thin film at a pH of 3.0 during deposition. Both hexagonal and cubic formations are observed when the value increases further to 3.5. Based on this finding, a pH of 3.0 will be considered the ideal solution for

this investigation since single-phase CdTe thin films were developed at this pH. The observed data's peak location and intensity match the file numbers 752083 and 800090 for cubic and hexagonal structures, respectively, that are used by JCPD. The peaks with (*) that show up at heat-treated peaks were associated with CdO.

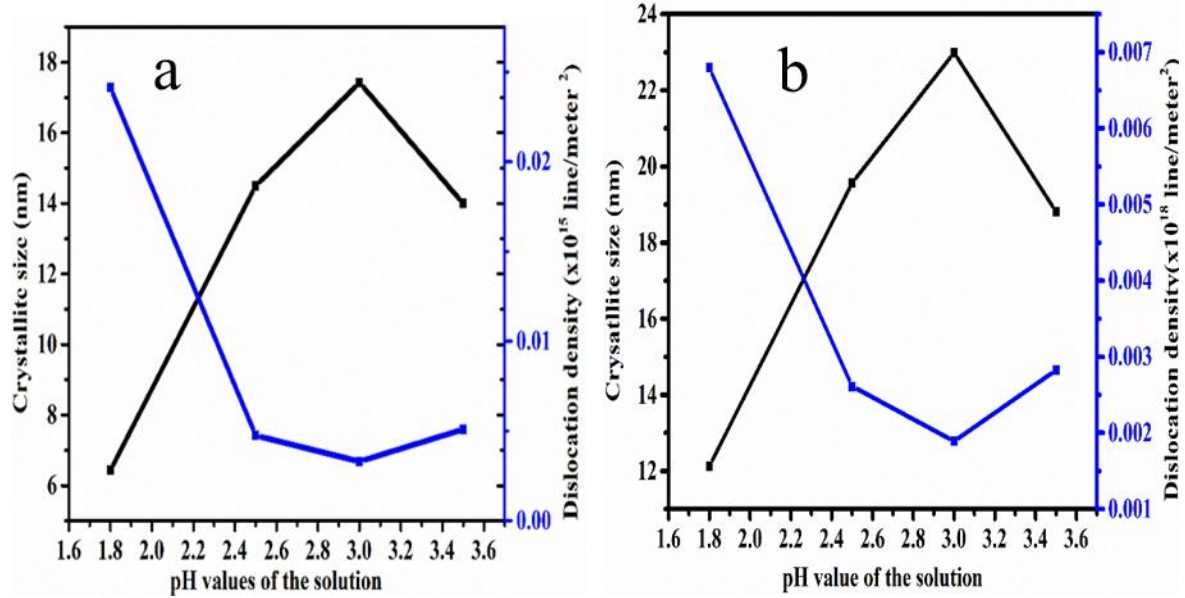


Figure 4. 7. Crystallite size and dislocation density as a function of different pH, (a) AD and (b) HT.

AD and HT samples' crystallite size and dislocation density values at various deposition pH levels are displayed in Figure 4.7 (a) and (b). According to the crystallite size analysis, the values vary with the pH of the deposition. The crystallite sizes measured were 6, 14, 17, and 14 nm, and the corresponding pH values were 1.8, 2.5, 3.0, and 3.5, respectively. Following HT, the crystallite size increased and was measured at 12, 20, 23, and 19 nm, with corresponding pH values of 1.8, 2.5, 3.0, and 3.5. The recrystallization of particles following heat treatment is the reason for this increase in crystallite size. With a deposition pH of 1.8 and 3.0, the maximum and minimum dislocation density values were recorded as 0.024 and 0.0033, respectively. The results of the dislocation density calculation also verified that the values changed with the deposition pH values. Heat treatment also lowers the dislocation density, with the highest and lowest values occurring at pH 1.8 and 3.0, respectively. Based on these findings, 3.0 is thought to be the ideal deposition pH for the creation of CdTe thin films.

4.2.2 Optical properties of CdTe with varying pH

The absorbance versus wavelength graphs for annealed and deposited samples are displayed in Figure 4.8 (a) and (b). It is discovered that the produced samples essentially absorb in the visible spectrum, and that the absorption rises as the pH of the deposition increases.

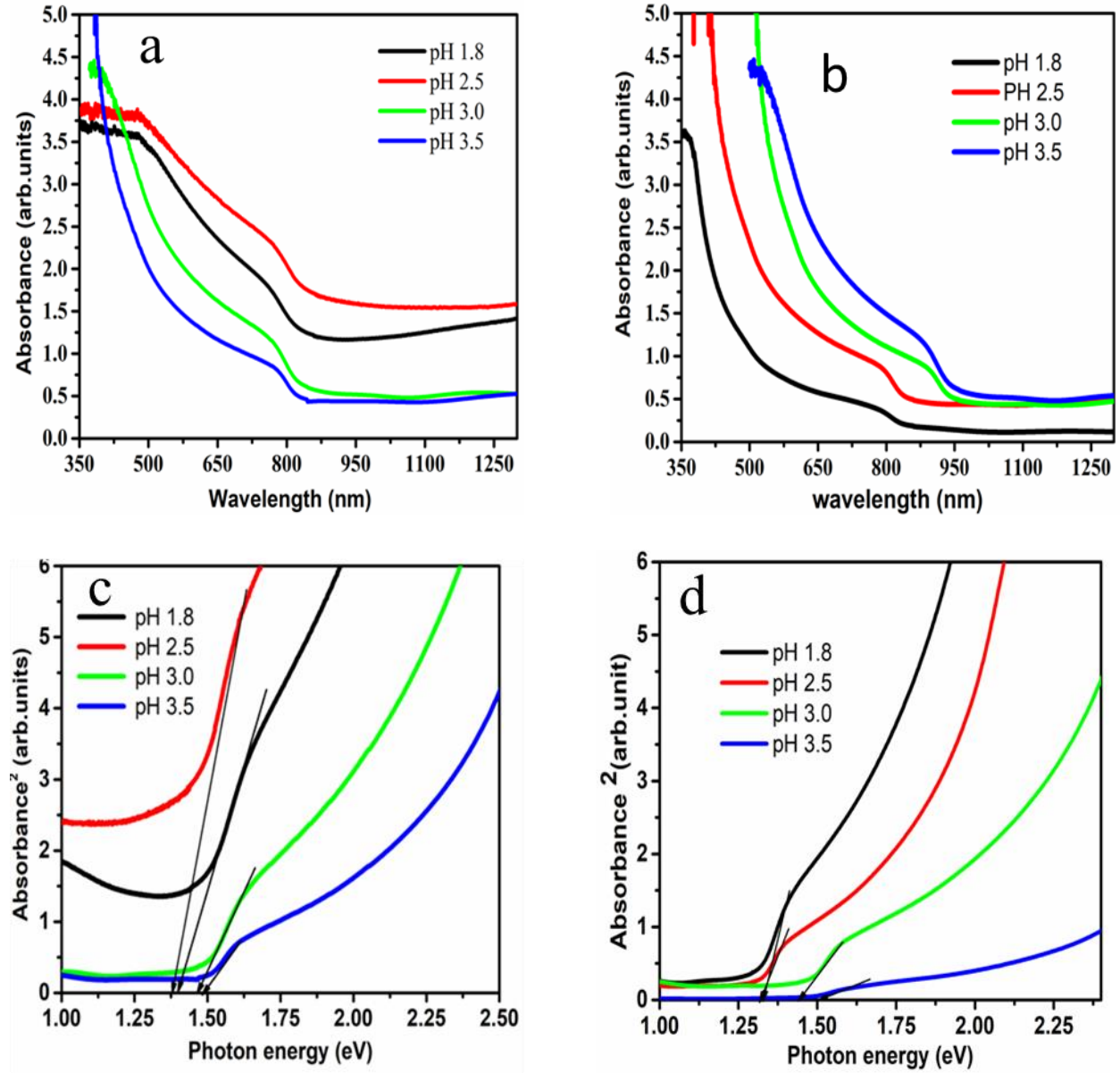


Figure 4. 8. Absorbance for CdTe films produced at varying pH levels as a function of wavelength (a) AD, (b) HT and the absorbance squared as a function of photon energy (c) AD. (d) HT

To find the energy gap values, it was reported in the literature that plots $(\alpha h\nu)^2$ against photon energy ($h\nu$) or uses Tauc plots (Chaure et al., 2003); (Chaure et al., 2004); (Sali & Chaure, 2021); (Ukarande et al., 2022); (Ukarande et al., 2023).

From the literature on ED thin films, the Dharmadasa IM group has discovered in this study program that very comparable findings are also obtained by plotting the square of optical absorption (A^2) vs photon energy ($h\nu$) (I. M. Dharmadasa, Madugu, et al., 2017b), (Olusola et al., 2015), (I. M. Dharmadasa, Echendu, et al., 2017), (Ojo & Dharmadasa, 2017).

Figures 3 (c) and (d) show the absorption squared (A^2) as a function of photon energy ($h\nu$) as-deposited and heat-treated samples. By extrapolating the straight line, the energy band gap was calculated by plotting a line tangent to the graphs to the photon energy axis at ($A^2=0$). The findings indicate that, for pH values of 1.8–3.5, the energy bandgaps were measured in the range of 1.38–1.58 eV for AD samples and 1.35–1.5 eV for HT. These results are consistent with those found in the literature (Yavorskyi et al., 2019).

The pH value plays a vital role in the ED of CdTe films, determining whether the resulting films are Te-rich or Cd-rich. At low pH values, Te-rich films form due to the reduced availability of Te^{2-} , while Cd-rich films can form at higher pH values as the deposition of Cd^{2+} becomes more favorable. This pH-dependent behavior is well-reported in the literature, where the challenge of achieving stoichiometric CdTe films is a common issue in ED. By understanding the relationship between pH and film composition, it becomes possible to fine-tune the ED process to produce films with the desired properties for specific applications, such as SCs, semiconductors, and detectors. According to published research, the majority of ED CdTe thin films from various sources suffer from Te-rich films as a result of growing at lower pH values (Yimamu, Afrassa, Dejene, Echendu, Terblans, et al., 2023b). This is because when Cd is removed from the surface by an acidic media, the film acts as Te-rich; conversely, when Te is removed by a basic medium, the film acts as Cd-rich CdTe (Shi et al., 2019). This study also shows this circumstance, which is consistent with the EDS findings. A decrease in the band gap was noted following HT. The primary intriguing finding of this discovery is that, for this acetate source the bulk CdTe energy band gap was 1.45 eV when the film was coated at pH 3.0 following HT. (Chu et al., 1995).

4.2.3. Surface morphology CdTe thin films

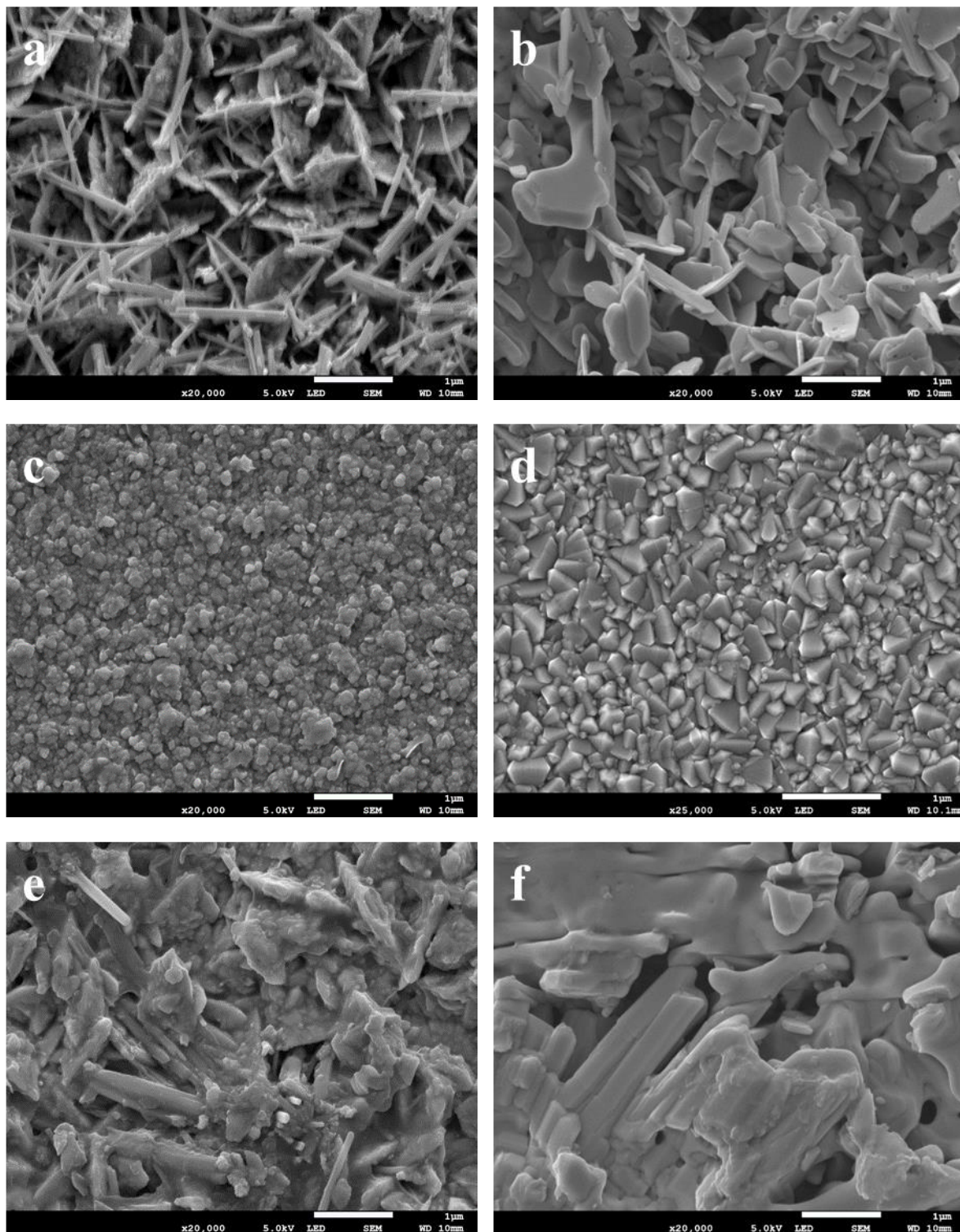


Figure 4. 9. The SEM images of CdTe thin films grown up at different pHs (a) pH 2.5 AD, (b) pH 2.5 HT, (c) pH 3.0 AD, (d) pH 3.0 HT, (e) pH 3.5 AD, and (f) pH 3.5 HT.

A basic understanding of surface properties are essential for optimizing thin-film SC fabrication. The surface of the thin film, which includes factors such as grain size, roughness, defects, and porosity, plays a great role in optical absorption, charge carrier transport, and interface quality. By carefully controlling surface morphology during deposition and post-deposition treatments, manufacturers can greatly enhance thin-film SC devices, increasing their efficiency and making them more viable for large-scale use in renewable energy applications. Figure 4.9 shows pictures captured by a scanning electron microscope (SEM) of AD CdTe thin films and HT grown at pH values of 2.5, 3.0, and 3.5 electrolytic solutions, respectively. It was observed that the films completely encased the substrate. The SEM pictures demonstrated how electrolytic pH levels significantly impact surface morphology, grain size, and shape. The post-deposition treatment altered the morphology. Te-rich CdTe developed and rod-like structures were seen when the film was grown at a pH of 2.5. Uniform and fairly spherical-shaped structures were seen when the pH of the deposition was 3.0, which is a good morphology than the others for the production of SC devices. The film exhibited a relatively homogeneous shape structure after being annealed at this pH. Agglomerated grains of different sizes and shapes were seen at a pH of 3.5. These results show that the pH of the electrolytic solution has a major effect on the production of CdTe thin films. Figure 1.18 makes it abundantly evident that the electrolyte pH affects the surface shape of the produced CdTe films and their potential uses. After annealing at a pH of 3.0, the film's surface seemed denser and more compact for potential use in SCs.

4.2.4. Electronic properties CdTe with pH

To confirm the conductivity of semiconductor thin films, such as CdTe films grown on conducting substrates like glass/FTO, it is crucial to assess their conductivity type. One effective method for this is through Photoelectrochemical Cell (PEC) measurements, which involve comparing the voltage under illumination to that in the dark. In this study, PEC measurements were performed on AD and HT CdTe thin films implanted at various pH values. The results, presented in Table 4.1, show that the PEC signal varied with pH. Specifically, films deposited at pH values of 1.8, 2.5, and 3.0 exhibited positive PEC values, indicating p-type conductivity of CdTe. Furthermore, the magnitude of the PEC signal decreased gradually as the pH of the deposition bath increased. The observation of p-type conductivity within this pH range suggests that the CdTe films are tellurium-rich (T-rich).

Table 4. 1 CdTe thin film (PEC) observations at various electrolytic pH

Electrolytic pH	V _L -V _D		Conductivity type	
	PEC Signal(mV)			
	As-prepared	Heat-treated	As-prepared	Heat-treated
1.8	72	65	P	p
2.5	45	41	P	p
3.0	14	-49	P	n
3.5	-6	-35	n	n

As the pH increased to 3.5, the deposited CdTe thin film exhibited n-type conductivity, indicating a cadmium-rich composition. However, after annealing, all the films exhibited p-type conductivity, which aligns with findings reported in other studies (Oluyamo et al., 2021b). The EDS analysis supports the conclusion that films deposited at lower pH values are tellurium-rich (T-rich), while films deposited at higher pH values, particularly at pH 3.5, exhibit a cadmium-rich (Cd-rich) composition. Additionally, these results are consistent with previous studies that have used various cadmium salts as the Cd source, further validating the relationship between deposition conditions, composition, and conductivity type in CdTe thin films (Shi et al., 2019)-(Razykov et al., 2009).

4.2.5. Surface Roughness Properties of CdTe

The surface morphology of CdTe thin films ED at different pH values significantly influences the film's roughness, impacting its optical and electrical properties. Scanning Probe Microscopy (SPM) is an essential technique for characterizing these surface features with high resolution. By carefully controlling the pH during ED and analyzing surface roughness, it is possible to tailor the films for improved photovoltaic performance, balancing light absorption and charge transport efficiency.

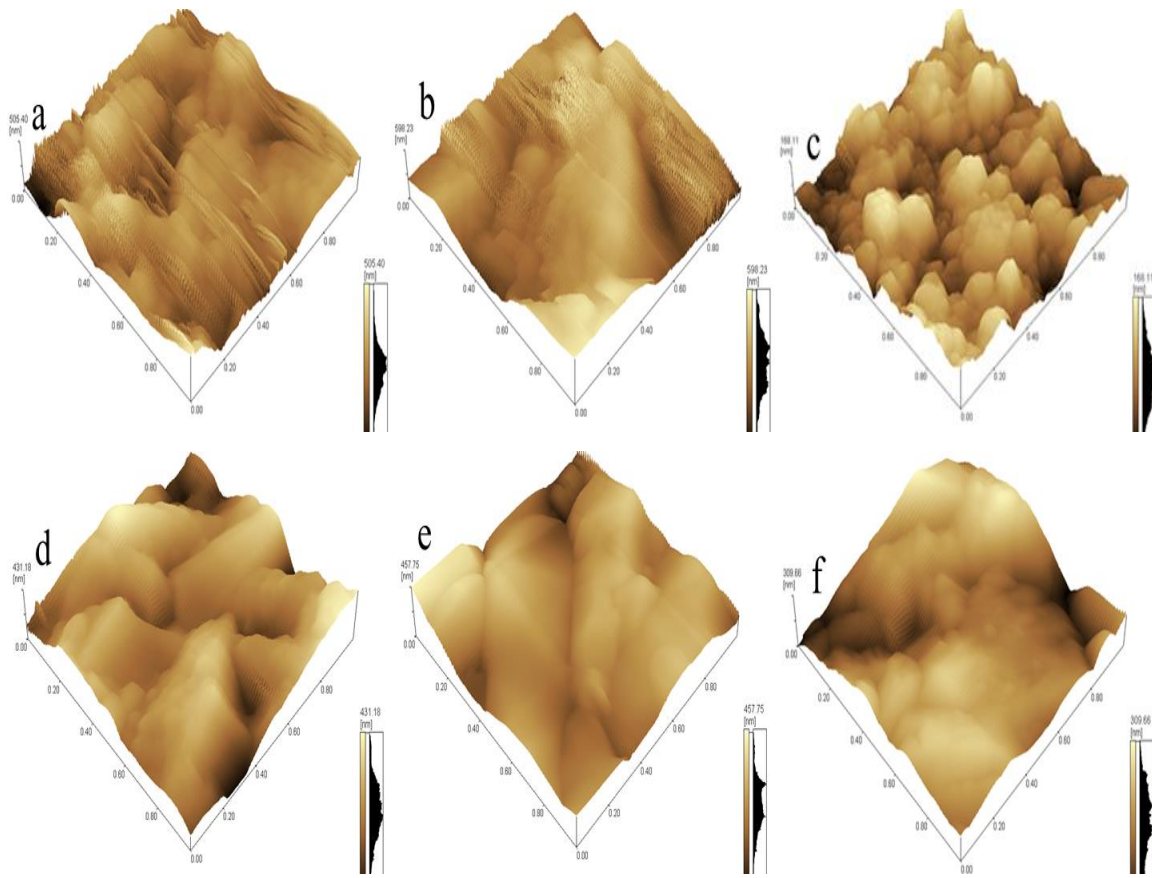


Figure 4. 10 The SPM images for the ED CdTe at different pH electrolytes (a) pH 2.5, (b) pH 3.0, (c) pH 3.5 and heat-treated (d) pH 2.5, (e) pH 3.0, and (f) pH 3.5.

As shown in Figure 4.10, As-prepared and heat-treated CdTe thin films that were produced at pH values of 2.5, 3.0, and 3.5 were chosen for further surface roughness and mean square surface roughness investigation. It is well-recognized that surface roughness impacts thin film optical transmission [38]. The optical path length of incident photons plays a crucial role, as high surface roughness can lead to total internal reflection, thereby increasing the likelihood of photon absorption. For a SC to achieve high efficiency, a surface with significant roughness is essential, as it enhances photon trapping and absorption. According to the current work's findings, the roughness changed when the pH of the deposition changed because of flaws or porosity in the films. The annealed samples with pH values of 2.5, 3.0, and 3.5 had average surface roughness values of 56.46, 78.73, and 47.17 nm, while the as-prepared samples had average surface roughness values of 50.08, 52.08, and 24.00 nm. An increase in average surface roughness was noted following heat treatment. The samples that were deposited and annealed at a pH of 3.0 had

the highest average surface roughness, making the film suitable for use as an absorber material in thin-film SE device applications.

4.2.6. Compositional Analysis of CdTe

The compositional characteristics of CdTe thin films made at various pH values were examined using energy-dispersive X-ray spectroscopy (EDS).

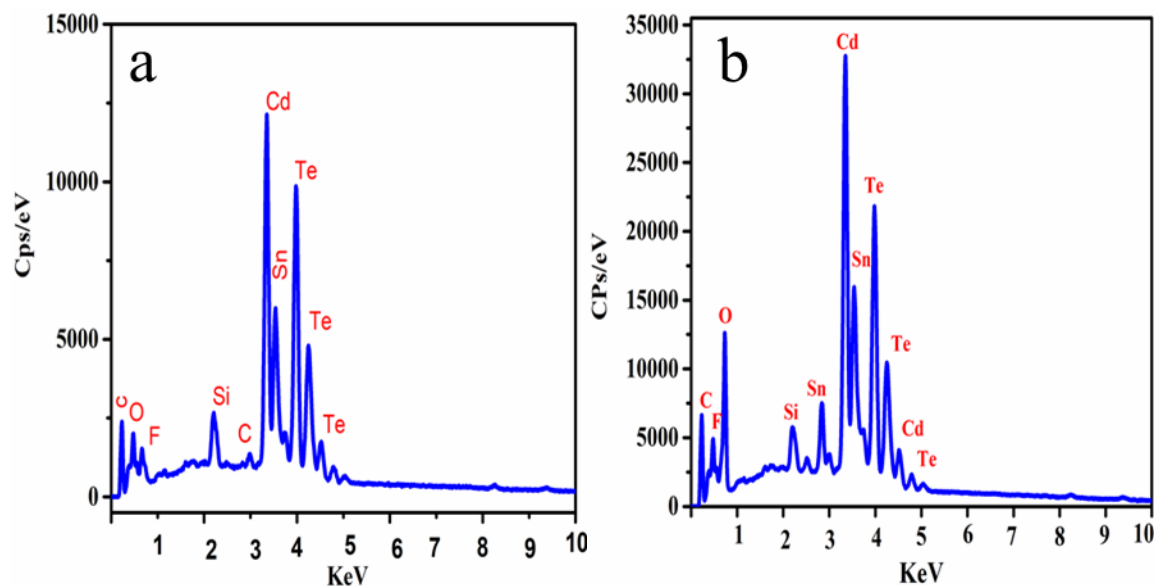


Figure 4. 11 . Representation of EDS spectra for CdTe at (a) pH 3.0 as prepared (b) pH 3.0 heat-treated.

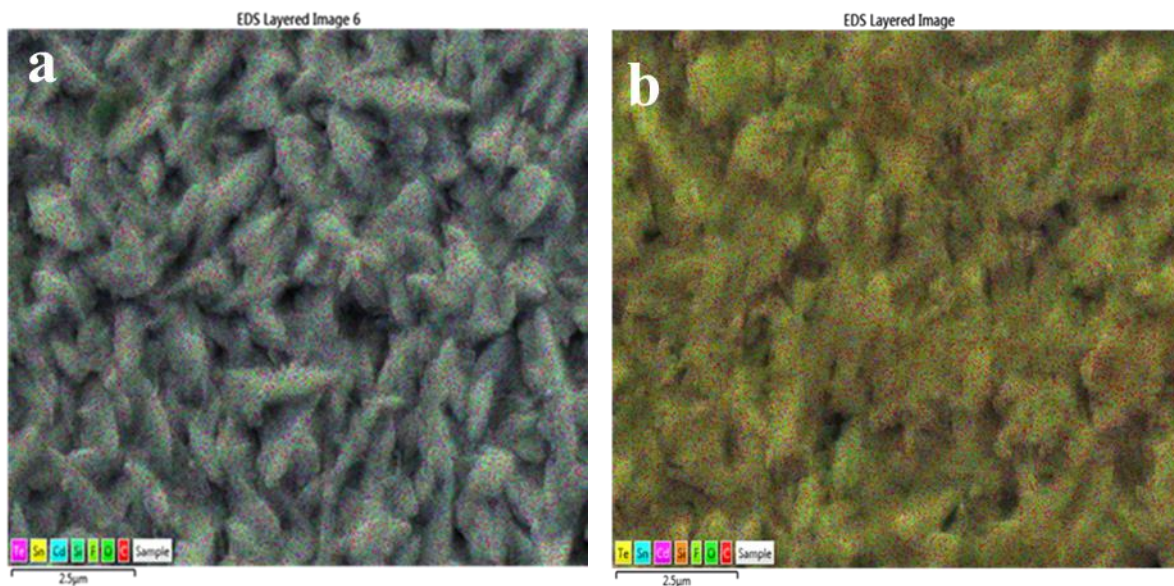


Figure 4. 12. The distribution of Cd and Te in the CdTe thin film at pH 3.0 as-prepared and (b) heat-treated sample.

The typical EDS spectra of CdTe thin films at pH 3.0 for the deposited and annealed samples are displayed in Figure 4.11 (a) and (b). Both the as-prepared and heat-treated CdTe thin film samples included the components Cd and Te, according to the elemental composition analysis.

Table 4. 2. CdTe thin films developed at various pH levels in terms of their elemental makeup.

electrolytic pH	Atomic%					
	As-prepared			Heat-treated		
	Cd	Te	Cd/Te ratio	Cd	Te	Cd/Te ratio
2.5	30	70	0.43	48	52	0.92
3	47	53	0.88	51	49	1.04
3.5	52	48	1.08	57	43	1.32

As shown in Table 4.2, the proportion of Cd and Te components changed as the pH changed. Both as-prepared and annealed samples show an increase in Cd and a reduction in Te in the film when the electrolyte's pH rises from 2.5 to 3.5. At a pH of 2.5, Te-rich CdTe was deposited after elemental Cd was spontaneously removed from the surface by the acidic solution

A substantial percentage of both Cd and Te was seen at a pH of 3.0 throughout the deposition process. The annealed Cd to Te ratio is 1.04, indicating a nearly stoichiometric composition. When the deposition pH was set at 3.5, Cd-rich CdTe was deposited, the Cd to Te ratio increased to 1.32, and the Cd % composition was greater. These results are in good agreement with those that have already been published (Ojo et al., 2021) (Saha et al., 2020).

4.3. Optimization of deposition voltage for CdZnTe

4.3.1. Structural properties of CdZnTe thin films

XRD was employed to analyze the structural characteristics of ED CdZnTe thin films. Figure 4.13 (a) Displays the XRD spectra of CdZnTe thin films produced at various voltages during deposition. The analysis results confirmed that cubic phases with polycrystalline nanomaterials were detected. The peaks are found at the angle of 24.10, 39.80, 46.97, and 62.8° with corresponding miller indexes of (111), (220), (311), and (331), respectively. There are peaks related to ZnTe at 31.00 and 33.26°, which is a cubic structure at (420) and (422), respectively.

These outcomes exhibit strong concurrence with JCPDS card no 752086 and 010582, respectively. Glass substrate (FTO)-related peaks have been observed at 26.92, 34.08, 38.69, 51.88, 54.91, 61.89, and 66.56°. Because FTO is annealed at a greater temperature and has a more crystalline

structure, its peaks are larger than those of films. The structural properties of CdZnTe were calculated using the equation (3.2-3.6).

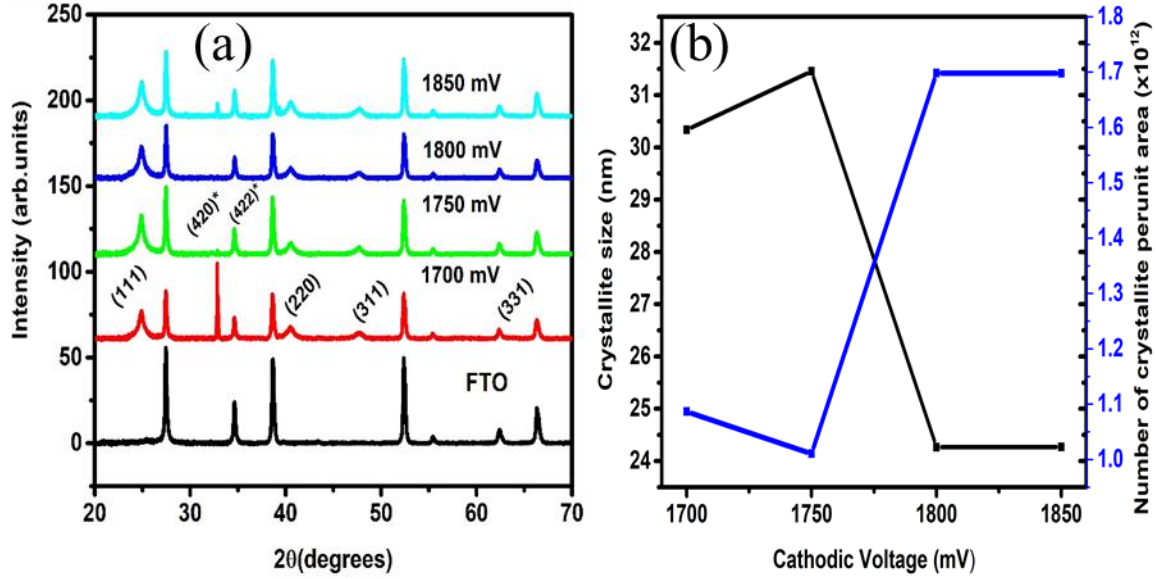


Figure 4. 13. (a) XRD Spectra of CdZnTe deposited at different cathodic voltage and (b) the D and N as a function of cathodic voltage.

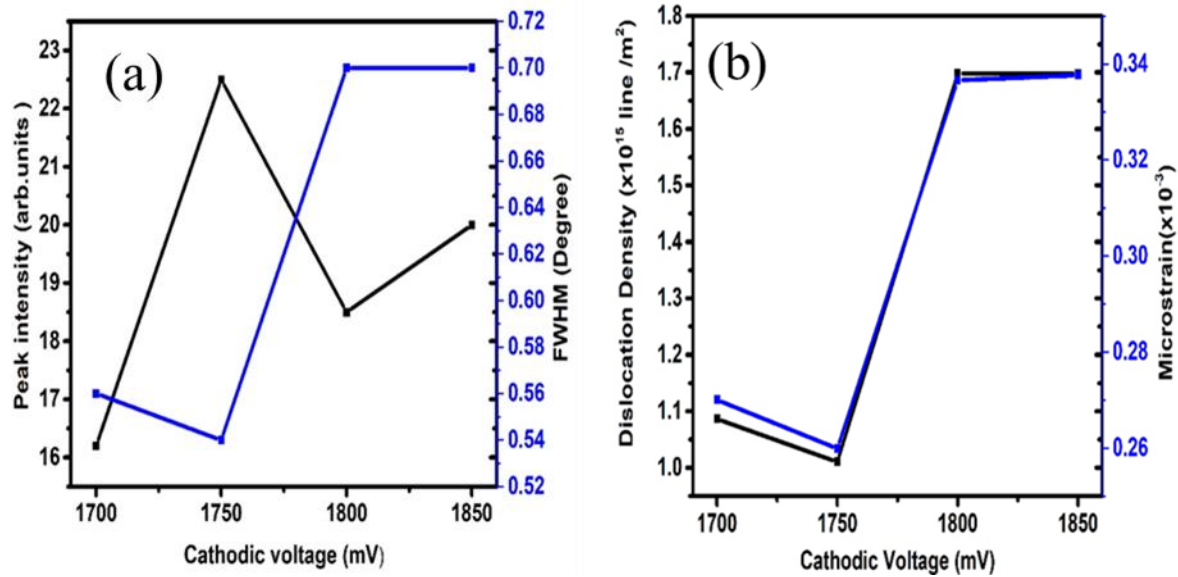


Figure 4. 14. (a) peak intensity and FWHM as a function of cathodic voltage and (b) δ and ϵ as a function of cathodic voltage.

Figure 4.13 (b) shows that the crystallite size and number of crystallites per unit area are functions of cathodic voltage. The analysis results showed that the crystallite size changed with cathodic voltage and recorded as 30.33, 31.46, 24.27, and 24.27 nm with deposition voltage of 1700, 1750,

1800, and 1850 mV, respectively. The maximum crystallite size was recorded at a deposition voltage of 1750 mV. The N was recorded as 1.086, 1.01, 1.69, and 1.69 with deposition voltages of 1700, 1750, 1800, and 1850 mV, respectively. The minimum number of crystallites per unit area was recorded at 1750 mV.

Figure 4.14 (a) Peak intensity and FWHM as a function of cathodic voltage. The results confirmed that the maximum peak intensity and lowest FWHM were taken at the voltage of deposition of 1750 mV.

Figure 2 (b) shows the dislocation density and microstrain as a function of cathodic voltage. The results indicate that the lowest dislocation density and microstrain were documented voltage of deposition of 1750 mV. The overall analysis confirmed that the cathodic voltage of 1750 mV is taken as the optimized voltage for forming CdZnTe thin films for optoelectrical applications.

4.3.2. Optical properties CdZnTe

The optical properties of CdZnTe thin films are crucial for their applications in optoelectronics and photovoltaics. UV-Vis was utilized to examine the optical characteristics of CdZnTe thin films that had formed.

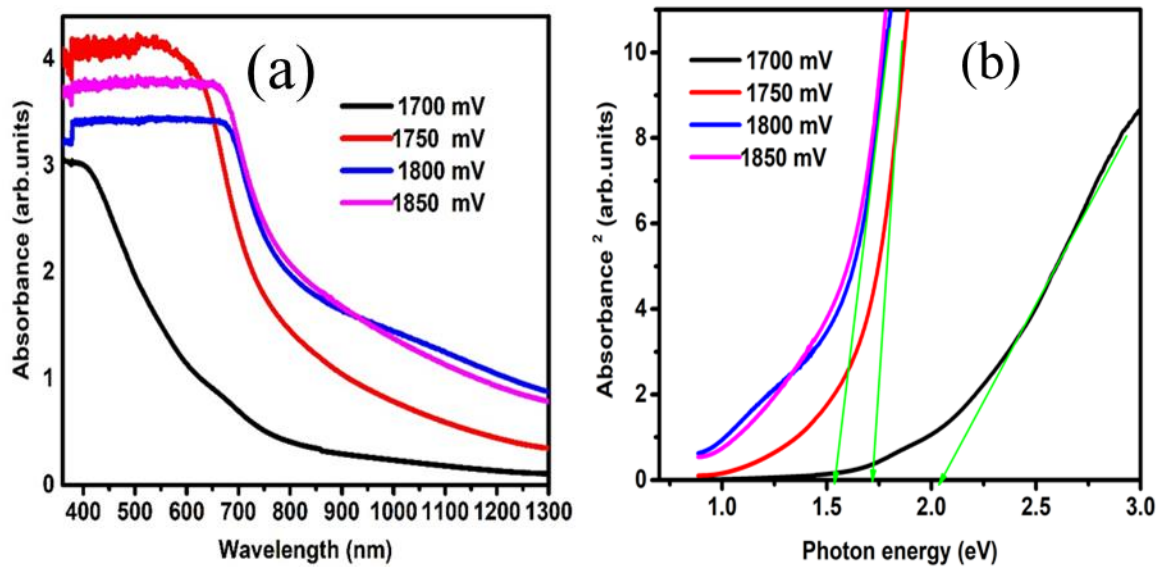


Figure 4. 15. (a) absorbance vs wavelength for CdZnTe thin film, (b) Absorbance square vs photon energy (eV).

Figure 4.15 (a) displays the wavelength-dependent absorbance spectra (nm). The optical absorbance has been measured wavelength region of 350 nm – 1000 nm. The result of the analysis confirmed the variation of absorbance with deposit voltage. The maximum near visible spectra region was noted at the voltage of deposition 1750 mV. The absorbance squared (A^2) in

conjunction with photon energy (eV) was displayed in Figure 4.15 (b). Band gaps were obtained by extrapolating the straight-line section to the photon energy axis ($A^2 = \text{zero}$). The energy band gap of the CdZnTe thin films that were ED was estimated from this investigation. Remarkably, figure 4.15 (b) offers a comparatively easy way to find. Similar to the relationship between $(\alpha h\nu)^2$ and photon energy, the energy bandgaps of thin-film nanocrystals. Both cases have the same energy bandgap value. Utilizing the A^2 vs. photon energy method has the advantage of removing the requirement to calculate the absorption coefficient (α) and ascertain the film thickness; therefore, $(\alpha h\nu)^2$ is not needed (Echendu et al., 2018).

It was noted that the energy band gap was documented as 2.05, 1.72, 1.55, and 1.55 eV with deposition voltages of 1700, 1750, 1800, and 1850 mV, respectively. The bulk band gap of ZnTe is 2.26 eV. Energy band gap differences between the films ranged from 1.55 to 2.05 eV. This increase in band gap is due to the quantum confinement phenomenon decreasing in crystalline size. It may be due to high pinhole formation caused by deposition voltage.

4.4. Effect of Zn-concentrations for CdZnTe

4.4.1. Structural Properties of CdZnTe thin films

The zinc concentration significantly influences the structural properties of ED CdZnTe thin films in the electrolyte. Figure 4.9 shows the XRD spectra of CdZnTe thin films with different Zn concentrations. The results presented in Figure 4.16 (a) and (b), as-deposited and annealed samples, confirmed that the presence of cubic structure CdZnTe thin films was detected. The material composition has a significant impact on the structural characteristics of thin films (Sharma et al., 2022). The results showed that preferential orientation (111) peak intensity increased as the concentration of Zn increased in both as-deposited and annealed samples, which enhanced crystal quality due to the film's increased Zn concentration (Kathalingam et al., 2021). The peaks are found at the angle of 24.10, 39.80, 46.97, and 62.8° with corresponding miller indexes of (111), (220), (311), and (331), respectively. There are peaks related to ZnTe at 31.00 and 33.26° which is a cubic structure at (420) and (422), respectively. These peaks are more visible when the films are annealed. These records demonstrate the films' polycrystalline composition. These results are in good agreement with JCPDS card no 752086 and 010582, respectively. Glass substrate (FTO)-related peaks have been observed at 26.92, 34.08, 38.69, 51.88, 54.91, 61.89, and 66.56°. The peaks for FTO are large when compared with films since they are annealed at higher temperatures and more crystalline. The crystallite size, dislocation density, and microstrain values from the

experimental results were varied within CdZnTe thin films with different concentrations of Zn, as tabulated in Table 4.3

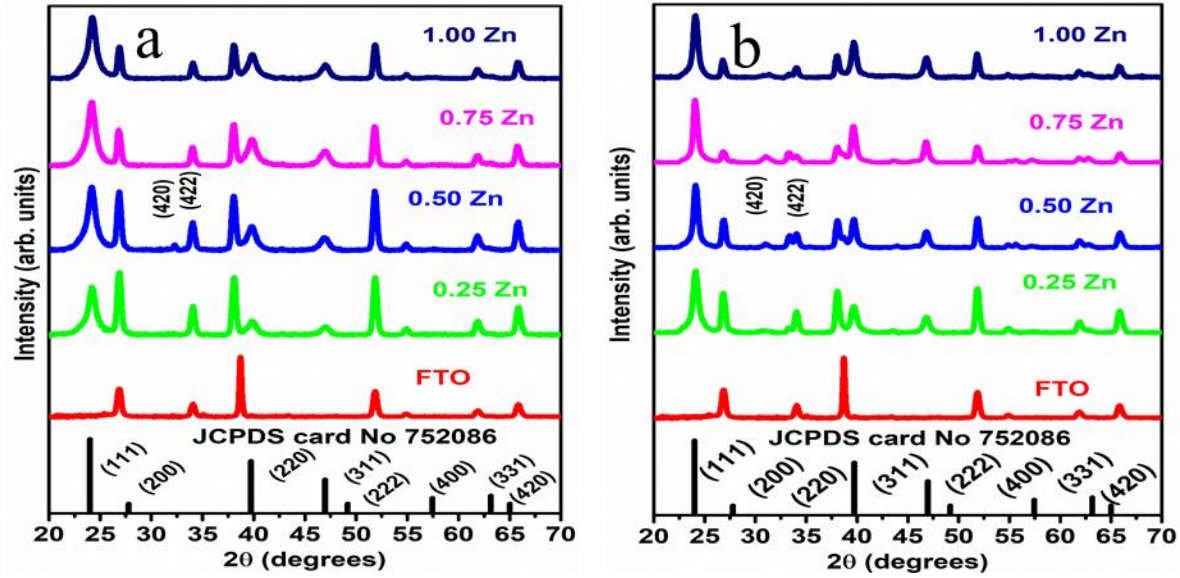


Figure 4. 16. XRD spectra of CdZnTe thin films: a) AD and b) HT

Table 4. 3. The structural properties of CdZnTe thin films

Zn Concentrations (M)	2θ		Crystallite size (D) nm		$\delta(\times 10^{15})$ line/m ²		$\epsilon (10^{-3})$	
	AD	HT	AD	HT	AD	HT	AD	HT
0.25	24.18	24.14 (111)	9.20	12.13	13.14	6.79	0.83	0.59
	39.89	39.68 (220)						
	47.03	46.82 (311)						
0.50	24.20	24.10	9.35	14.94	11.43	4.48	0.77	0.48
	39.84	39.68						
	46.92	46.84						
0.75	24.22	24.06 (24.03)	9.13	14.93	11.98	4.48	0.79	0.48
	39.80	39.66 (39.74)						
	47.01	46.78 (46.97)						
1.00	24.25	24.10	8.91	13.39	12.58	5.57	0.81	0.54
	39.89	39.68						
	46.97	48.86						

showed that the crystallite size D was varied with Zn concentration, and the maximum was recorded at 0.50 Zn concentration 9.35 nm for as-deposited samples, which are in the quantum dot range. For annealed samples, the crystallite size increased for 0.50 Zn Concentration, which is 14.94 nm. This is due to the small particles recrystallized to create large crystallites throughout the annealing process, as evidenced by the increase observed after annealing. The dislocation density of CdZnTe was varied from $(11.43-12.58) \times 10^{14}$ line/m² for as-prepared samples and $(4.48-6.79) \times 10^{14}$ line/m² as annealed samples with (0.25, 0.50, 0.75, 1.00) M Zn concentrations.

The microstrain values were changed with both AD and HT samples with $(0.77-0.83) \times 10^{-3}$ for AD and $(0.48-0.59) \times 10^{-3}$ with annealed samples with (0.25, 0.50, 0.75, 1.00) M Zn concentrations.

4.4.2. Optical properties of CdZnTe with Zn-Concentrations

The optical measurements of ED CdZnTe thin films were performed by using UV-VIS spectroscopy. Figures 4.17 (a) and (c) show the absorbance of CdZnTe thin films as a function of wavelength (nm) as-deposited and annealed samples, respectively. The result shows that the absorbance was varied with Zn concentration. The maximum absorbance was recorded when 0.50 M of Zn was added, and the minimum was recorded at 0.25 M Zn for as-deposited films. For annealed samples, the absorbance increases with Zn concentration near the visible spectral region.

The bandgap of CdZnTe thin films was calculated using absorbance square as a function of photon energy. The band gap was estimated by extrapolating the tangent line to the graph with the x-axis. It is possible that these thin films could be used in SCs due to their increasing transmittance (Altiokka & Yildirim, 2018).

The effect of Zn in energy band gap engineering of CdZnTe thin films was investigated in this section since ZnTe has a higher energy band gap than CdTe, the addition of Zn for the band gap of CdZnTe thin films was investigated.

Figures 4.17 (b) and (d) show the absorbance square as the function of photon energy in calculating the energy band gap. The energy band gap was recorded as deposited 1.82, 2.02, 2.07, and 2.12 eV with 0.25, 0.50, 0.75, and 1.00 M Zn concentration, respectively. The results showed that the energy band gap increased as Zn concentration increased because CdTe has an energy band gap of 1.45 eV and ZnTe has 2.25 eV. The energy band gap for annealed samples was recorded as 1.52, 1.63, 1.71, and 1.75 eV with 0.25, 0.50, 0.75, and 1.00 M Zn, respectively. The band gap was increased with Zn concentrations. It was observed that the energy band gap was reduced after annealing due to increased crystallite size and the removal of vacancy and pinholes during the annealing effect. These energy band engineering of CdTe and ZnTe thin films will have potential applications for back metal contact or absorber layer in thin film SE

conversion. The results of the study are consistent with earlier published research (Chaure et al., 2004)(Kathalingam et al., 2021)(Bansal & Rajaram, 2005).

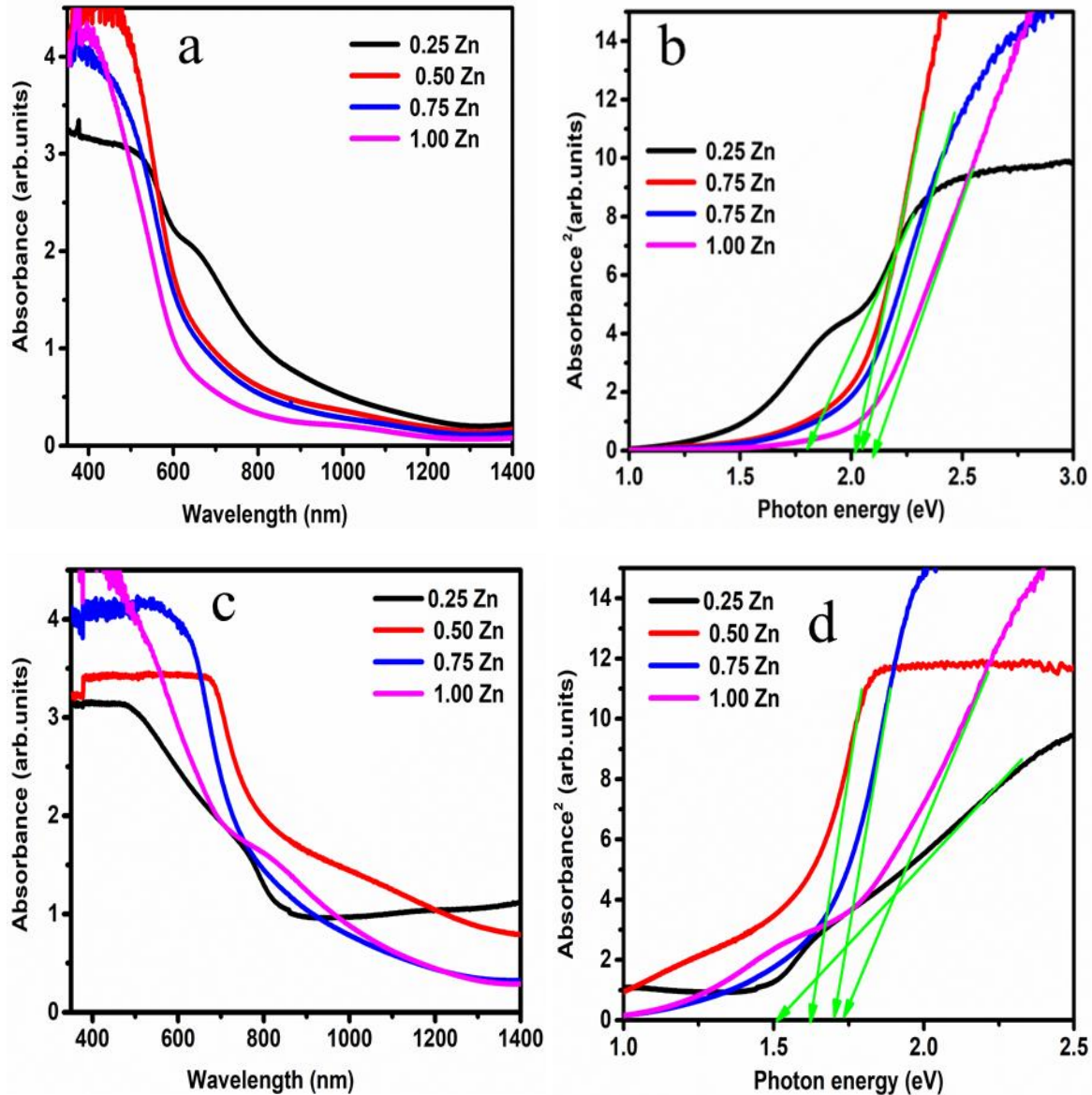


Figure 4. 17. The absorbance at the function of wavelength a) as-deposited and b) energy bandgap as-deposited, c) absorbance for annealed samples, and d) energy band gap for annealed samples.

4.4.3. Surface morphological properties CdZnTe with Zn-concentrations

The surface morphological properties of ED CdZnTe thin films at different properties of Zn were characterized by using scanning electron microscopy (SEM). As figure 4.18 shows the image for CdZnTe thin films at different Zn concentrations were observed. The result confirmed that the grain size and shape of films were affected by the concentration of Zn.

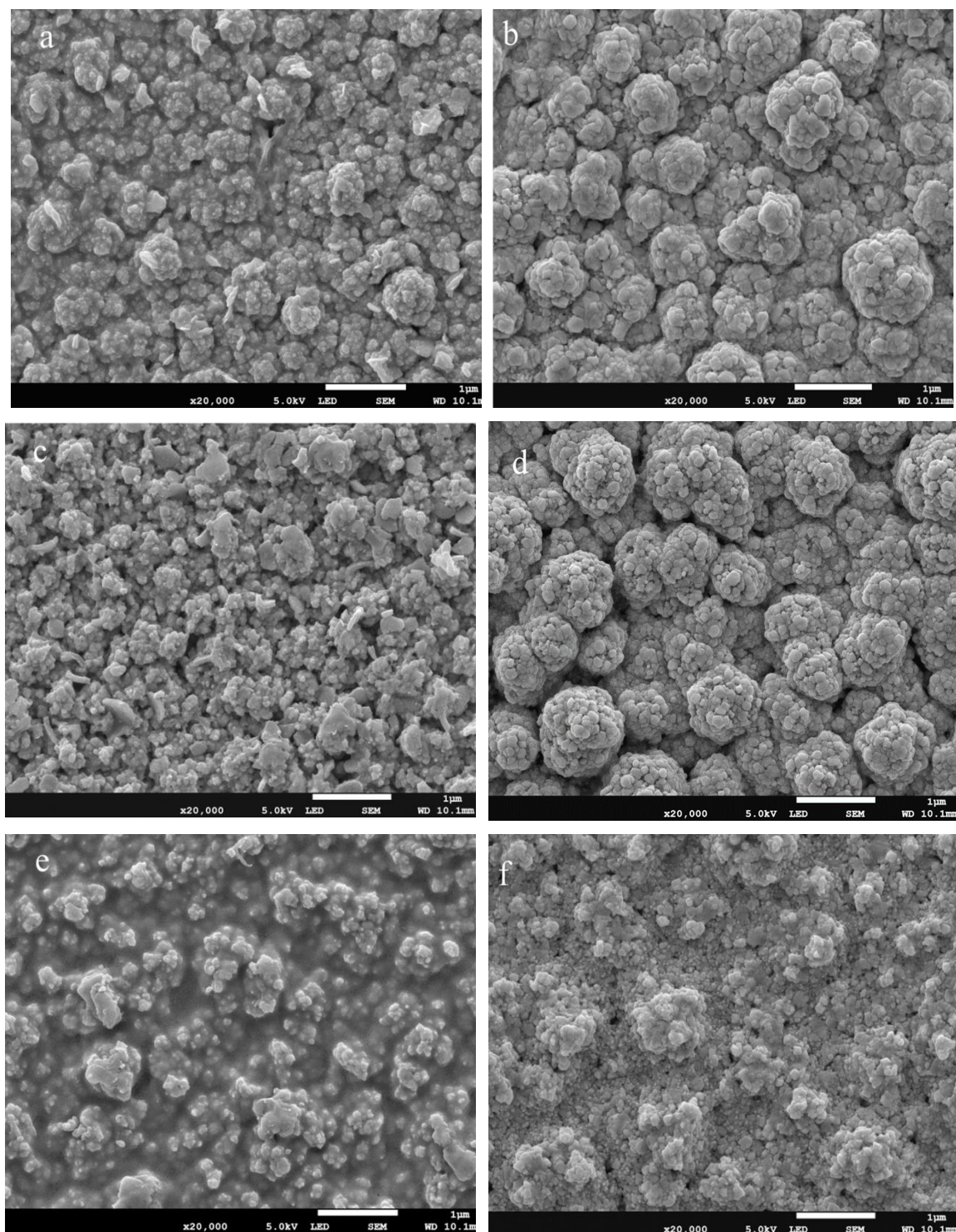


Figure 4. 18. The SEM image for ED of CdZnTe at different concentrations of Zn a) 0.25 M as-prepared, b) 0.25 M as-annealed, c) 0.5 M as-prepared, d) 0.5 M as-annealed e) 1 M as- prepared f) 1 M Zn annealed.

The results showed that the agglomerated small grain size is observed for as-deposited thin films when 0.25 M Zn was added. For annealed samples, the increments in grain size were observed due to the recrystallization of small grains to large grain sizes during the annealing process. To maximize the absorption of sunlight for the most efficient one-band gap p-n junction PV device, a surface morphology free of pinholes and voids is necessary to apply SC absorber layers (Yimamu, Afrassa, Dejene, Echendu, Terblans, et al., 2023b). When the 0.5 M Zn was added, a uniform morphology was observed in both as-deposited and annealed samples. When the concentration of Zn is 1M, very small agglomerated grains were detected in both as-prepared and annealed samples. From the SEM result, $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Te}$ thin films have a good morphology for SE applications as absorbers or back contact materials.

4.4.4. Surface roughness properties CdZnTe

The surface roughness properties of ED CdZnTe thin films were characterized by using Scanning probe microscopy (SPM). One important topic is the study of thin-film materials' surface roughness, particularly for SCs and other technical applications (Werta, State, et al., 2019).

Figure 4.19 (a-f) image results showed that R_a and mean square surface R_q varied with the concentration of Zn as both as-prepared and annealed samples. The study of average surface roughness is very important since it is directly related to photon absorption on the film surface; the higher the roughness, the higher the absorbance (Yimamu, Afrassa, Dejene, Echendu, Terblans, et al., 2023b). In this study, SPM findings verified that the R_a properties of CdZnTe thin films were recorded as 45.45, 52.15, and 47.12 nm with growth voltage of 1700, 1750 and 1800 mV, respectively. It has been found that films with excellent transmission spectra have low surface roughness, more effective homogeneity, and crystallites (Malkas et al., 2014). Larger grains, however, provide easier electron movement with less scattering and have fewer grain borders, which is advantageous for SC devices (Abdul-Manaf et al., 2015). From our analysis result, the films produced with a voltage deposition of 1750 mV are suitable for the absorber layer for SC devices, and this voltage will be taken as the optimized voltage for CdZnTe thin films.

. The incident light beam was less scattered by low roughness (Altioikka & Yildirim, 2018). These findings strongly demonstrate that surface roughness has a significant impact on Zn concentrations.

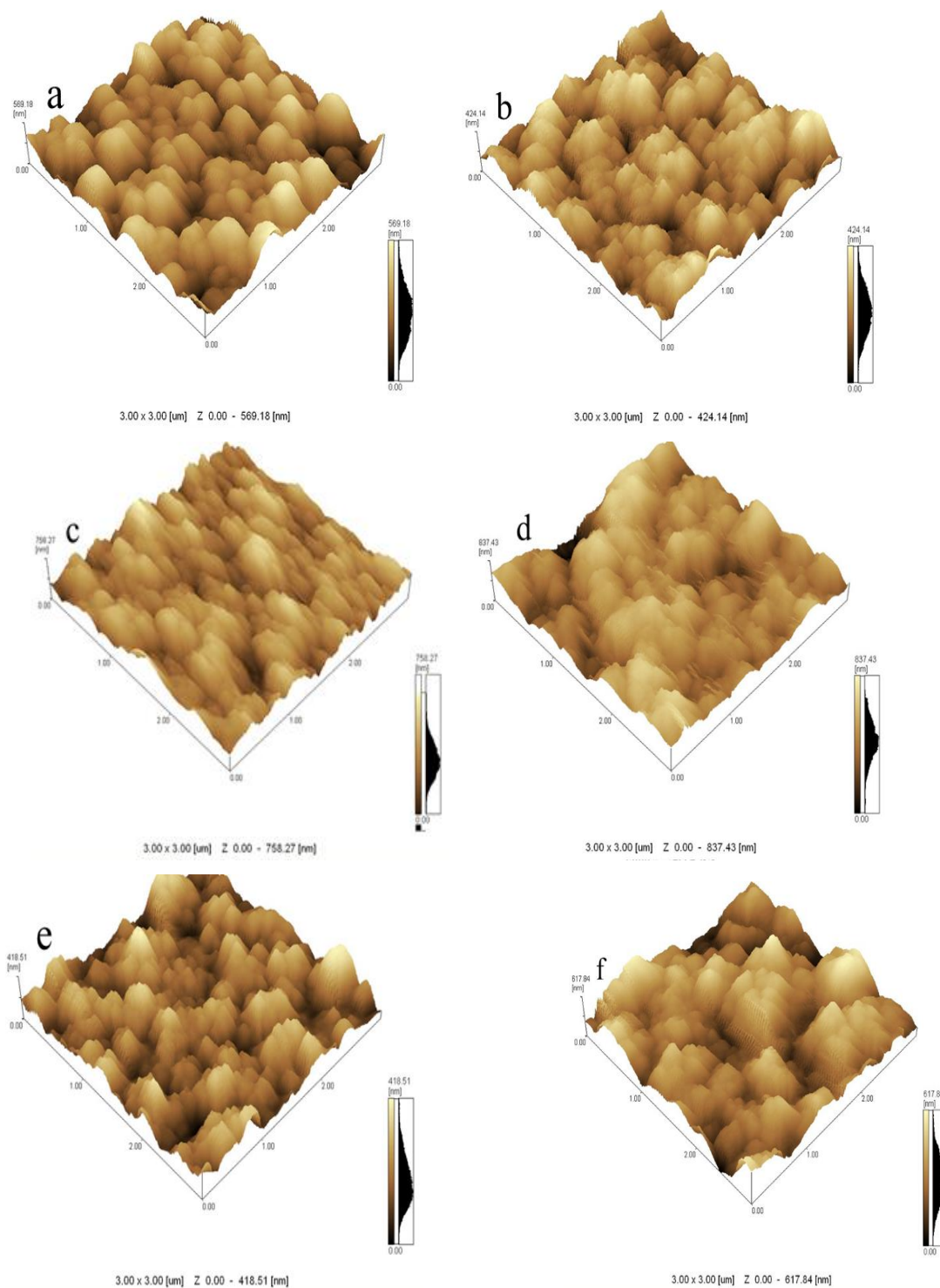


Figure 4. 19.SPM image for CdTe thin films with different concentrations of Zn a) 0.25 m Zn as-prepared, b) 0.25 m Zn as-annealed, c) .5 m Zn as-prepared, d) 0.5 m Zn annealed e) 1 m Zn as-prepared f) 1 m Zn as-annealed.

The R_a and R_q were recorded as-deposited at 0.25 M Zn 78.68 nm and 95.89 nm and 56.79 nm and R_q 69.76 nm annealed samples. For 0.50 M Zn for as-deposited R_a 75.79 nm and R_q 94.23 nm and annealed R_a 92.06 nm and R_q 114.01 nm for 1 M Zn R_a 55.54 nm and R_q 68.75 nm as-deposited samples and for annealed R_a 85.31 nm and R_q 105.74 nm. The R_a and R_q values are increased from 0.25 M Zn to 0.50 M Zn and decreased to 1 M of Zn, and when the samples are annealed, the surface roughness is increased. The maximum surface roughness was observed when 0.50 M Zn was added. Which is used as an absorber material for SE applications. A high-efficiency SC device requires the highest level of roughness because it increases the optical length of the incident photon due to the increased likelihood of photon absorption caused by total internal reflection at high roughness (K. S. Rahman et al., 2019)(Kaushalya et al., 2018)(Patel et al., 2018) or back contact for SE conversation applications.

4.4.5. Compositional Properties CdZnTe

The elemental composition of ED CdZnTe thin films undergoing quantitative analysis was characterized by energy-dispersive X-ray spectroscopy (EDS). The result showed in Figure 4.20 that all the desired elements, Cd, Zn, and Te, were detected. The percentage composition of each element was varied with Zn concentrations. The peaks related to F, Si, O, and Sn were from the FTO glass substrate, and C was from the carbon double-tape used during SEM measurements. The analysis confirmed with optical analysis that the concentration of Zn increases in the reverse direction Cd reduced. The main aim is to reduce Cd toxic elements and substitute environmentally friendly Zn.

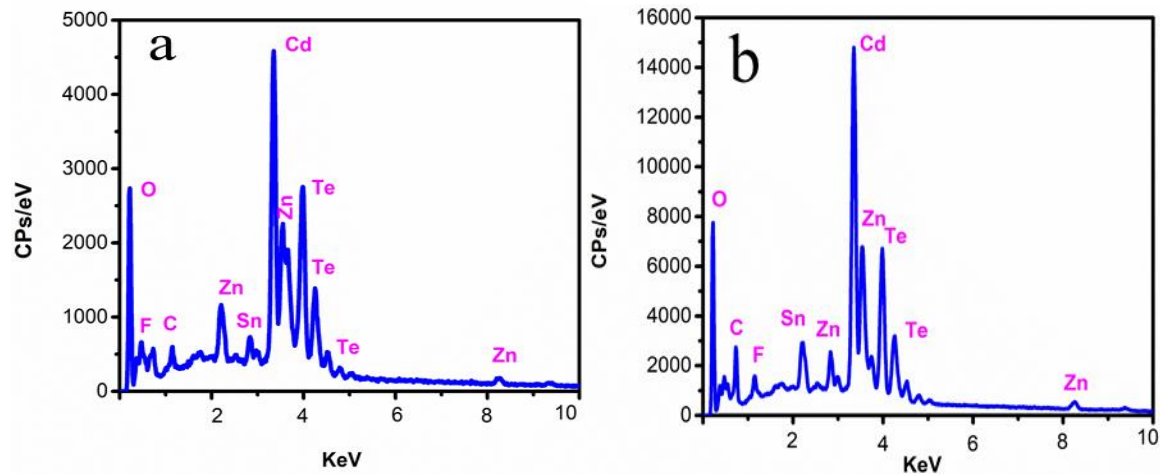


Figure 4. 20. The EDS spectra of $Cd_{0.5}Zn_{0.5}Te$ a) AD and b) HT samples

4.5. Optimization of deposition voltage for CdMgS

4.5.1. cyclic voltammetry measurement (CV)

For the formation of CdS: Mg thin films, 400 ML of deionized water have been combined with 0.3 M of cadmium chloride ($CdCl_2$), 0.06 M of magnesium chloride ($MgCl_2$), and 0.03 M sodium

thiosulphate ($\text{Na}_2\text{S}_2\text{O}_3$). The study focuses on optimizing the growth voltage for CdS: Mg thin films since it is crucial in identifying the film's crystallinity, excellence, and suitability for various applications such as photovoltaics or optoelectronics. The initial findings suggested that a deposition voltage of 1455 mV provided the best crystallinity, which led to further investigation using smaller voltage intervals around this value to fine-tune the deposition conditions. Ultimately, this optimization process will help produce films with the highest possible quality and performance for their intended applications.

Figure 4.21 displays the current density against the cathodic voltage graph, also known as the cyclic voltammetry measurement (CV). An ion's reduction potential is crucial to ED activities since it establishes the circumstances and viability of ED. The typical reduction potential (E°) is around -0.403 V for Cd^{2+} ions to reduce to Cd metal, -2.37 V for Mg^{2+} ions to reduce to Mg metal, and +0.448 V for sulfide ions S_2 to elemental S. (Yimamu, Dejene, et al., 2024), (Salim, Olusola, et al., 2015), (I. M. Dharmadasa, Madugu, et al., 2017a), (Yimamu, Afrassa, Dejene, Echendu, Terblans, et al., 2023b), (A. E. Alam et al., 2019).

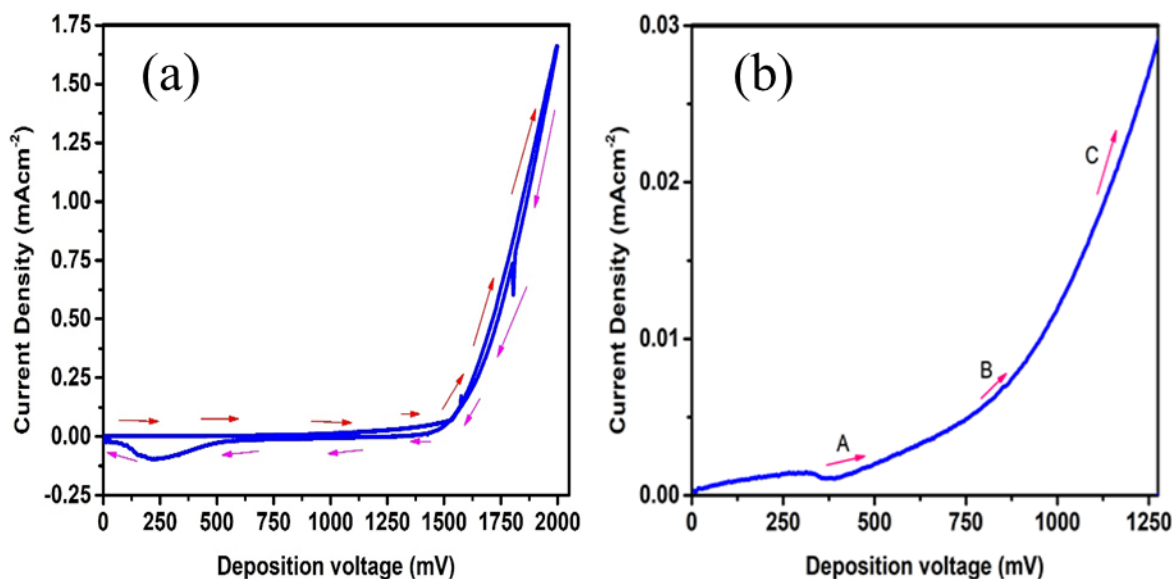


Figure 4. 21. The CV graph for CdS: Mg with 0.3 M CdCl_2 , 0.06 M MgCl_2 , and 0.03 M $\text{Na}_2\text{S}_2\text{O}_3$ was used. (b) Forward CV plot in voltage region from 0- 1250 mV.

The reduction potentials of various elements are essential in establishing the ideal parameters such as voltage, current density, and electrolyte composition needed for effective thin-film ED.. Elements like sulfur (S), which possess positive reduction potentials, can be readily deposited on glass/ITO substrates. Cadmium ions, with a relatively favorable reduction potential, can also be

reduced effectively under appropriate electroplating conditions. In contrast, magnesium (Mg) has a more negative reduction potential, signifying that it demands higher energy to be reduced than cadmium. Therefore, careful optimization of deposition voltage is essential to achieve thin films that closely match the desired stoichiometric composition. As illustrated in Figure 4.21, cyclic voltammetry (CV) measurements were conducted within the 0–2000 mV range to attain the optimum voltage for deposition. The current density during ED is primarily affected by factors such as the composition of the electrolytic source, growth temperature, and the applied voltage. Elemental sulfur (S) began to accumulate at a cathodic voltage of around 400 mV, corresponding to region A in Figure 4.21(b), due to its relatively higher positive reduction potential, as indicated by the forward cycle in the figure. The growth of Cd started when the applied voltage was raised to 700 mV, as observed in region B of Figure 4.21(b). Co-deposition of Cd and S took place at this time, resulting in the formation of an S-rich CdS layer. Further increasing the cathodic voltage to 1150 mV triggered the deposition of magnesium (Mg) on the ITO substrate, as shown in region C of Figure 4.21(b).

CV analysis reveals that the applied voltage between 1300 and 1525 mV is optimal for the initial CdS: Mg films growth.. This voltage window was identified as the most effective for synthesizing films with the desired composition and structure. Based on these findings, further preliminary depositions were conducted within this voltage range to fine-tune the deposition process. Specifically, deposition voltages of 1300, 1355, 1410, 1455, and 1525 mV were chosen to produce magnesium (Mg)-doped thin films. These voltages were selected to systematically evaluate the impact of varying cathodic potentials on the film's characteristics, such as composition, morphology, and structural integrity. This approach allows for precise control over the synthesis of CdS: Mg films, ensuring the achievement of the desired doping levels and material properties. This step refers to the initial analysis conducted on the properties of the CdS: Mg thin films. The crystallinity and X-ray diffraction (XRD) peak intensity are typically two important parameters used to characterize the quality of thin films.

Crystallinity refers to how ordered or well-structured the crystal lattice is in the film. A high crystallinity means that the thin film has a well-organized atomic structure, which usually results in better electronic and optical properties. XRD peak intensity measures the intensity of specific diffraction peaks, which correspond to particular planes in the crystal structure. A higher intensity typically indicates that more of the material is in a crystalline form, and the peaks are sharper,

which suggests fewer defects in the crystal structure. In this case, it is observed that the film grown at a cathode voltage of 1455 mV exhibited the uppermost crystallinity and the maximum XRD peak intensity. This implies that 1455 mV is the optimal voltage at which the film formed with the best crystalline structure and highest diffraction peak intensity, suggesting good film quality at this specific voltage.

For optimizing the Deposition Voltage after the preliminary analysis shows that 1455 mV yields the best film quality (in terms of crystallinity and peak intensity), the next step is to optimize this voltage to further refine the film quality. To do this, five CdS: Mg thin films are deposited at various cathode voltages (Vg), specifically around 1455 mV. The voltages are chosen at intervals of 5 mV. By varying the voltage in such small increments, the aim is to identify the precise voltage where the film exhibits the highest possible quality, not just in terms of crystallinity and peak intensity but potentially in terms of other properties like structure, surface roughness, optical transparency, and morphology.

4.5.2. Structural Properties of CdMgS thin films

Figure 4.22(a) presents the Grazing Incidence X-ray Diffraction (GIXRD) spectra of electroplated CdS: Mg thin films deposited at various cathodic voltages. The data confirm that the films exhibit a hexagonal polycrystalline structure, which is characteristic of CdS: Mg thin films. Two prominent diffraction peaks, corresponding to the (100) and (101) lattice planes, are observed at 2θ values of 24.88° and 28.17° , respectively. Additional diffraction peaks are also detected, corresponding to the (002), (110), (103), (112), (201), and (104) planes, with 2θ values of 26.52° , 43.76° , 47.92° , 51.81° , and 52.76° , respectively.

The intensity of these peaks varies depending on the cathodic voltage used during deposition. At a voltage of 1445 mV, the (100) and (101) peaks exhibit relatively low intensity. However, when the applied voltage is improved to 1450 mV, the peaks reach maximum intensity. As the deposition voltage is further raised, the peak intensities begin to decrease, although a slight increase in intensity is detected at 1465 mV. This variation could be attributed to the increased addition of magnesium (Mg) into the CdS lattice, which may alter the crystallinity and phase structure of the films. The patterns acquired are in wonderful alignment with the standard JCPDS card number 75-1545, which corresponds to the hexagonal structure of CdS with the space group $p6_3mc$ (186). These findings align well with findings that have already been published in the scientific literature ((Werta et al., 2024)(Gangawane et al., 2021). The majority of CdS ED formed hexagonal crystals

suitable for application in SC technology. The CdS unit cell's structure is depicted in Figure 2(b), the 2x2x2 super cell CdS structure in Figure 4.8(c), and the CdS: Mg structure in Figure 4.10(d).

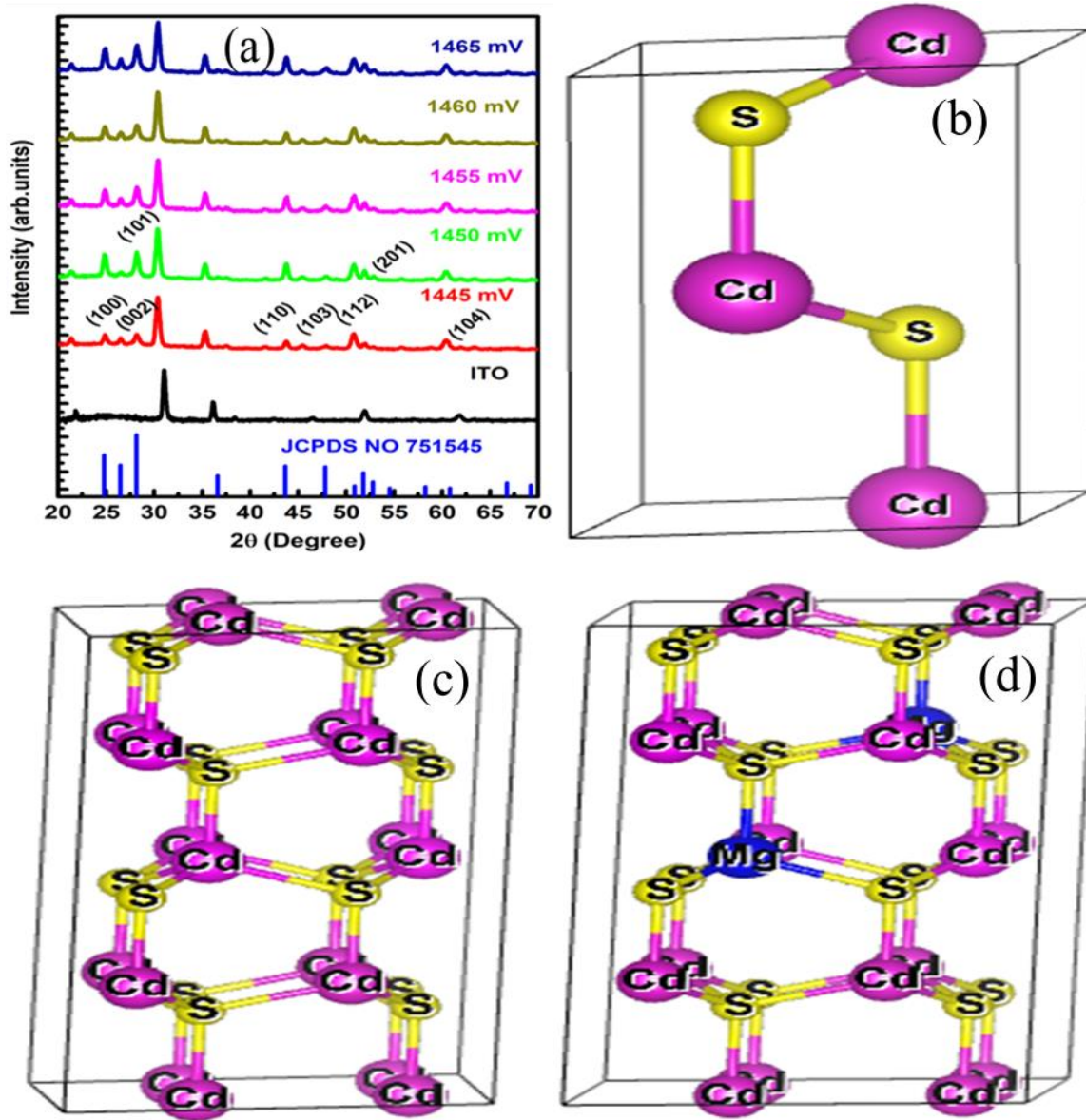


Figure 4. 22. (a) GIXRD plot of ED CdS: Mg thin films synthesized at various Voltage (b) CdS unit cell structure (c) CdS supercell structure (d) CdS: Mg structure

The hexagonal structure of CdMgS with lattice constants of $a = 4.15 \text{ \AA}$ and $c = 6.74 \text{ \AA}$ is seen in the figures 4.22. Because magnesium has lower atomic radii than cadmium, it replaces cadmium. Given that the dopant ions (Mg^{2+}) have smaller ionic radii ($0.72 \text{ \AA}$) than the host ions Cd^{2+} ($0.97 \text{ \AA}$) and S^{2-} ($1.84 \text{ \AA}$), it is anticipated that the lattice parameter values are going to decline with doping. This could be due to changes in the inherent strain of the crystals generated by defects and

lattice deformations (Sivaraman et al., 2016). These findings significantly lessen the problem of lattice mismatch between CdS and CdTe in CdTe/CdS heterojunctions, which are widely used in applications such as SCs (Kapadnis et al., 2020).

The favored (101) peak was used to compute the structural variables for ED thin films. Where all are Miller indices of the diffraction peak under consideration. Figure 4.23 (a) shows the FWHM values and the relationship between crystallite size and coating voltage. Fig. 4.23 (b) displays the microstrain and dislocation density as a function of the coating voltage. Peak analysis findings showed that FWHM values changed with deposition voltage, with the lowest and greatest values at 1445 and 1450 mV being 0.57 and 1.3, respectively. At deposition voltages of 1445, 1450, 1455, 1460, and 1465 mV, the ED CdS: Mg thin films' crystallite sizes were measured to be 6.57, 15.00, 12.57, 10.69, and 12.95 nm, respectively. Figure 4.11 (b) shows how increasing the coating voltage alters the dislocation density and microstrain values. For 1445 and 1450 mV deposition voltages, the highest and lowest dislocation density values are 23.11 and 4.44×10^{15} line/m², respectively. The study of the microstrain value verified that the lowest value was observed at a coating voltage of 1450 mV. In addition to the greatest peak intensity, the largest crystallite size was measured at 1450 mV. According to this investigation, 1450 mV is the ideal voltage.

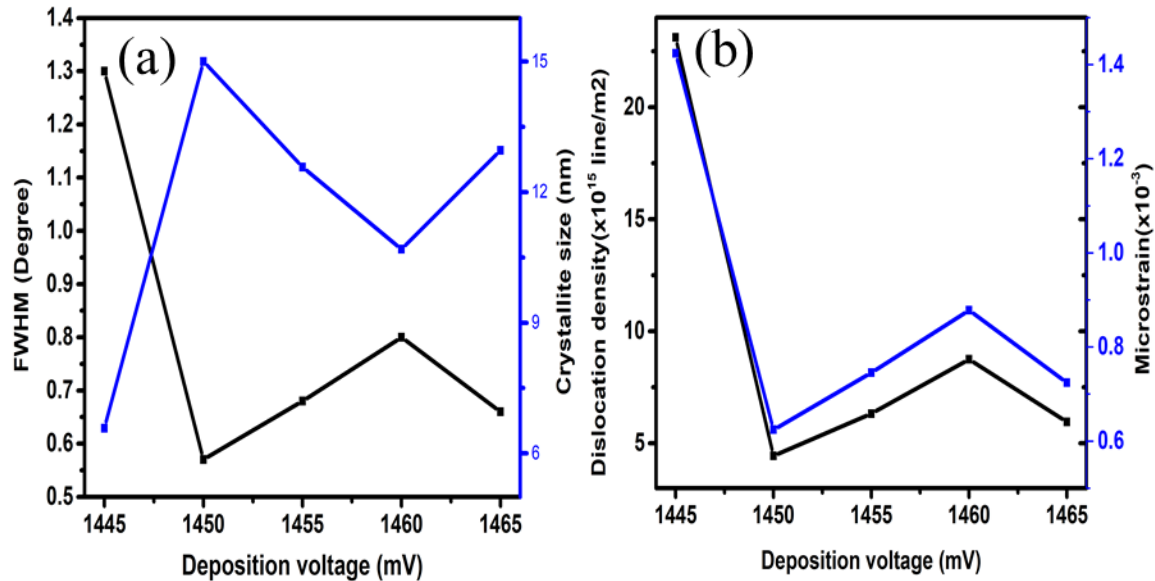


Figure 4. 23. FWHM and Crystallite size as a function of deposition voltage (b) dislocation density and microstrain as a function of deposition voltage.

4.5.3. Optical Properties of CdMgS

The optical characteristic of CdS: Mg thin films formed on glass substrates covered with ITO was examined using UV-VIS spectrophotometry, which was carried out at wavelengths ranging from

300 to 1000 nm. Figure 4.24 (a) and (b) show the transmittance and absorbance Vs wavelength and the absorbance squared vs of photon energy (eV) is shown in Figure 4.14 (c).

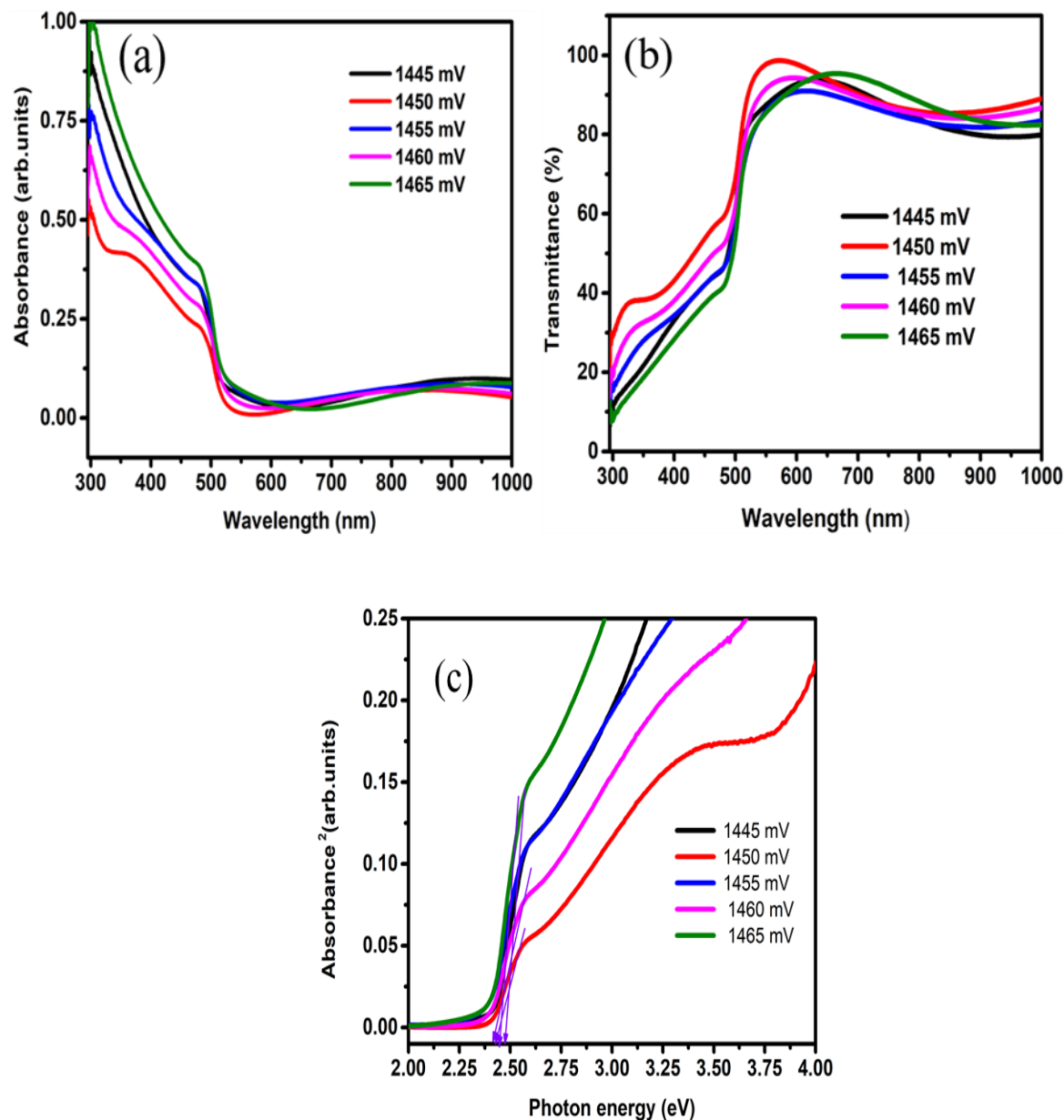


Figure 4. 24. (a) The absorbance and transmittance are a function of wavelength (b), and the square of absorbance (A^2) is a function of photon energy.

Variability with growth voltage is evident in the transmittance and absorbance findings. At a growth voltage of 1450 mV, the highest transmittance and lowest absorbance in visible spectra were recorded, making the film developed at this specific voltage more appropriate for use in SCs as a window or buffer layer. The figure's straight-line graph is being extrapolated. The films' band gaps are obtained by comparing 4.24 (c) to the photon energy axis ($A^2 = 0$). The energy band gap

of the ED CdS: Mg thin films was calculated using these graphs. Notably, the graph of the A^2 vs photon energy offers a somewhat easy way to find the energy bandgaps of thin film semiconductors, much like the case of $(\alpha h\nu)^2$ vs. photon energy. In both cases, the energy bandgap value is the same. Using the A^2 vs. photon energy approach has the advantage of removing the requirement to calculate the absorption coefficient (α) and identify the film thickness, therefore $(\alpha h\nu)^2$ is not necessary (Echendu et al., 2018). At deposition voltages of 1445, 1450, 1455, 1460, and 1465 mV, the energy band gap of CdS: Mg thin films was measured at 2.45, 2.44, 2.46, 2.48, and 2.47 eV, respectively.

4.5.4. Raman Spectroscopy study of CdMgS

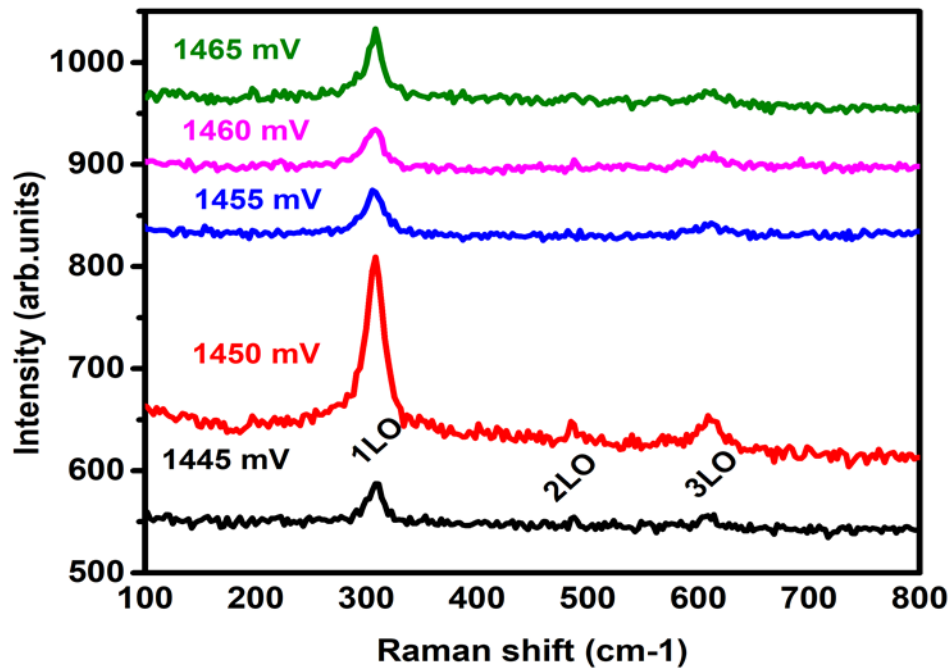


Figure 4. 25 Raman spectra of CdS: Mg thin film grown using ED methods at varying deposition voltages

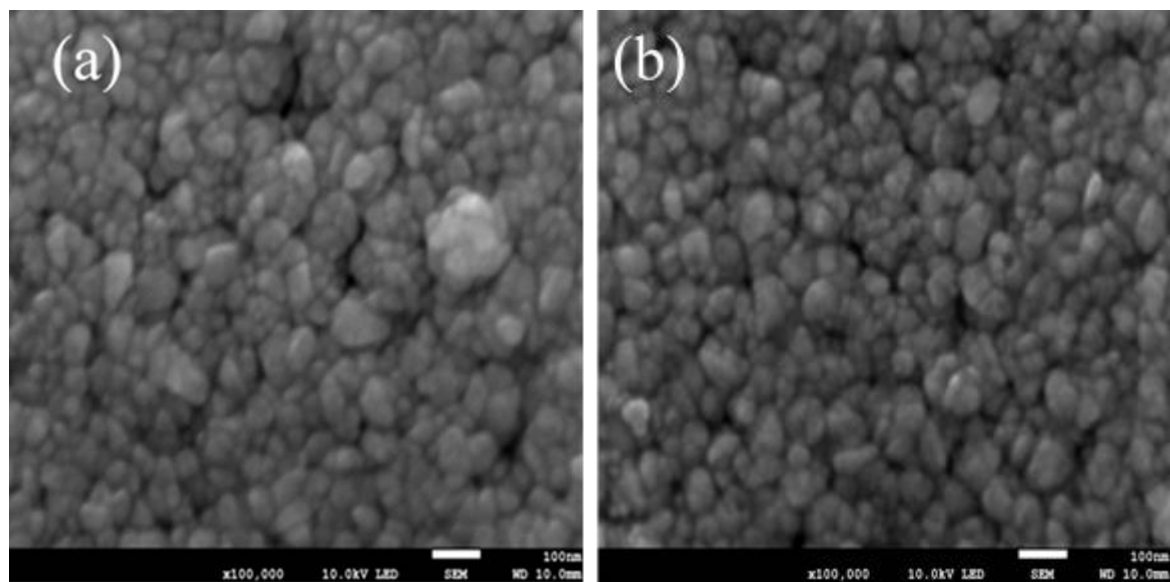
An efficient system for analyzing vibrational, rotational, and other low-frequency modes in a system is Raman spectroscopy (RS). It provides information on molecular vibrations, which is helpful for characterizing and identifying materials. The basis of RS is the inelastic scattering of monochromatic light by molecules, often from a laser.

The Raman spectra of CdS:Mg thin films made by ED techniques at different deposition voltages are displayed in Figure 4.25. The outcome verified that the longitudinal optic (1LO) phonon vibration's prominent peak was observed at wave numbers of 306 cm^{-1} . With observed wave numbers of 486 cm^{-1} and 612 cm^{-1} , respectively, the other two longitudinal optics are the second

longitudinal optic (2LO) and the third longitudinal optic (3LO). Raman spectroscopy, measuring the material's crystallinity, non-crystallinity, or amorphous phase, is as easy as examining the properties of the system (rotation, vibration, and other low-frequency modes). In order to examine the crystallinity of CdS: Mg thin films, RS has been used to support XRD studies. As the deposition voltage changed, so did the shift's strength. At 1445 mV, the minimum was observed, indicating poor crystallinity. The highest intensity was measured at 1450 mV for the deposition voltage. As the growth voltage increased, the Raman peak intensity dropped to around 1465 mV. The outcome demonstrates that compared to films applied at various voltages, the film formed at 1450 mV is more crystalline. The XRD examination revealed the same situation. Thus, there is good agreement between the RS and XRD analyses. This outcome aligns with earlier research findings in the literature(M. F. Rahman et al., 2020).

4.5.5. Surface morphology CdMgS thin films

The SEM pictures of ED CdS: Mg thin films produced at various deposition voltages are displayed in Figure 4.26.



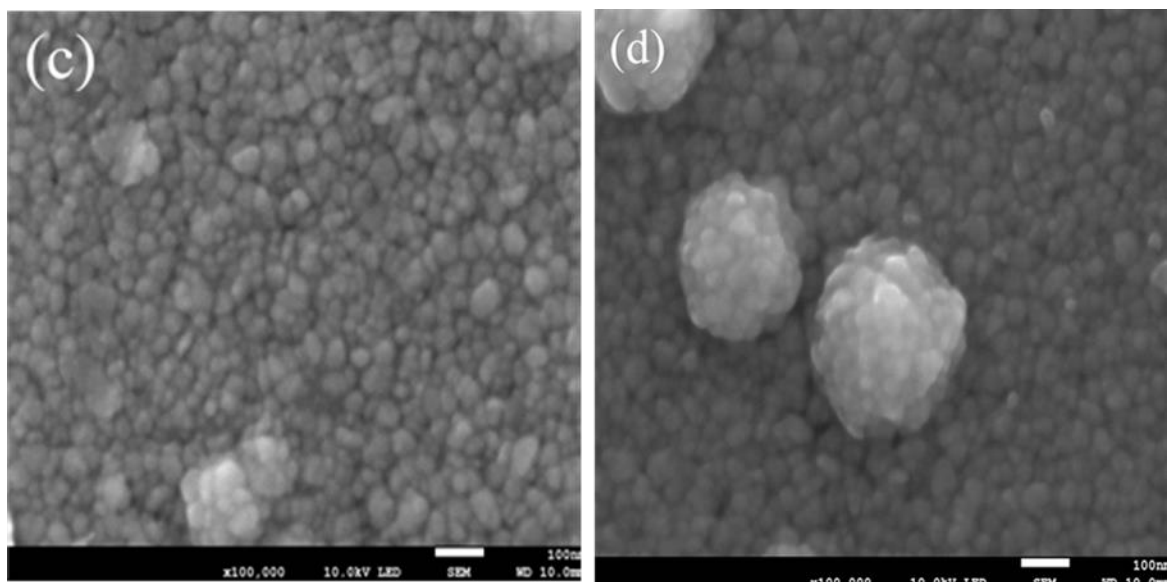


Figure 4. 26 SEM images of ED CdS: Mg thin films deposited at (a) 1445 mV, (b) 1450 mV, (c) 1455 mV, and (d) 1460 mV.

The findings verified that as the cathodic voltage rose from (1445- 1460) mV, the surface morphology of the films changed. When the film was placed at 1445 mV, an uneven surface was seen. The voltage of 1450 mV produced large, homogeneous grains. Additionally, as the image illustrates, raising the 1455 mV results in smaller grains; the sample created at 1450 mV showed more consistent substrate coverage. The surface of CdS: Mg films is greatly influenced by their formation, shape, adhesion, and quality (El-rouby & Aliyev, 2014).

4.5.6. Surface roughness properties of CdMgS

SPM is a terrific instrument for exploring a material's surface features. It provides essential details on the uniformity and texture of thin films and makes it possible to sketch the layout of the film surface (Kumari, Suthar, Himanshu, Kannan, et al., 2022). Figure 4.27 shows the SPM spectra of ED CdS: Mg thin films produced at different deposit voltages. R_q and R_a of the ED CdS: Mg thin films changed in response to the coating voltage. The R_q values are 6.37, 4.07, 9.41, 16.10, and 21.88 nm for the matching voltages for deposition of 1445, 1450, 1455, 1460, and 1465 mV, respectively, and the R_a values are 9.63, 5.61, 16.07, 19.30, and 27.93 nm for the deposition voltages of 1445, 1450, 1455, 1460, and 1465 mV, respectively.

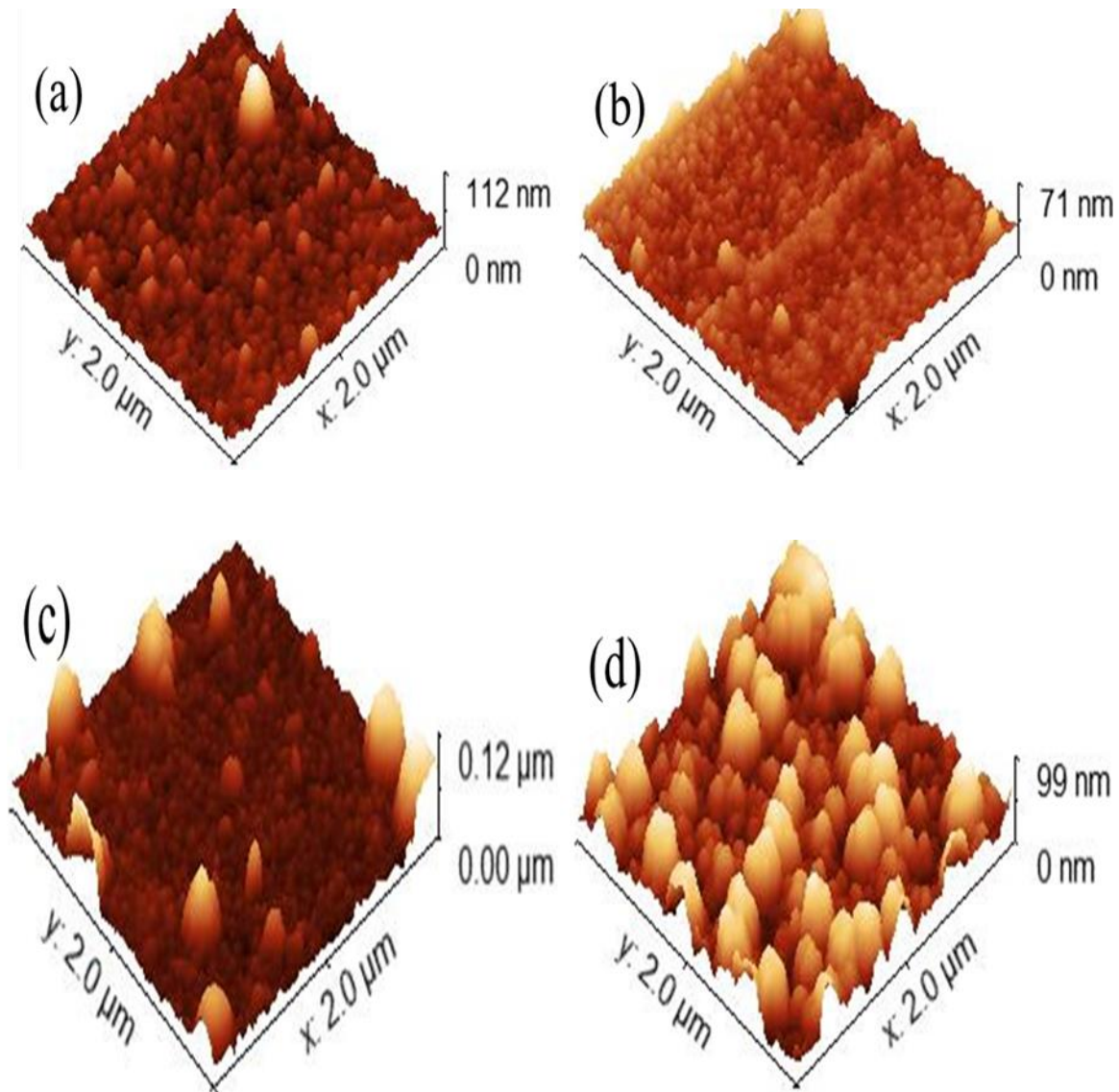


Figure 4. 27 The SPM spectra of Ed CdS: Mg thin films grown at different deposition voltages (a) 1445 mV, (b) 1450 mV, (c) 1455 mV, and (d) 1460 mV.

According to the results, the smallest R_q and R_a were measured at a growth voltage of 1450 mV. This means the film formed at this voltage is better suited as a window material for thin-film SC systems that use CdTe. The roughest surface indicates more light absorption on the surface, and window absorption loss results from the absorption of light in the window layer not always contributing to photo-current generation in SCs. The film developed at a voltage of 1450 mV has a greater chance of being used as a window or buffer layer in the production of SCs since the lowest surface roughness has less light absorption.

4.5.7. Compositional Study Analysis CdMgS

EDS examinations were performed on ED CdS: Mg thin films made on ITO substrate to confirm the elements present on the film and ascertain the percentage of each element. One effective technique for determining a material's elemental makeup.

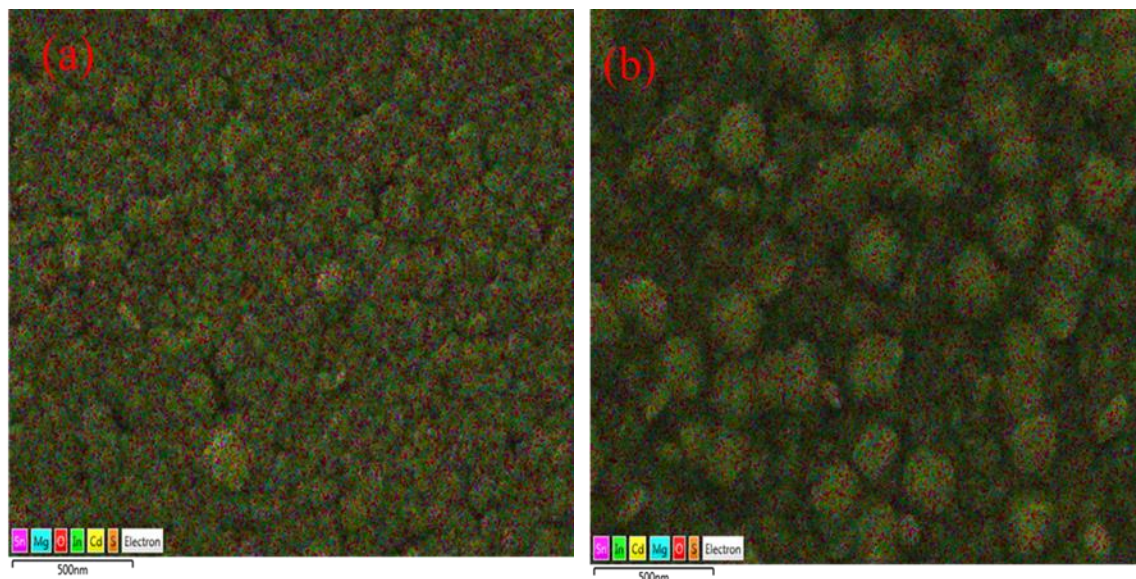


Figure 4. 28. Representative EDS mapping of ED CdS: Mg thin films (a) 1450 mV and (b) 1460 mV.

Table 4. 5. Elemental composition analysis of CdS: Mg thin film

Deposition voltage		Atomic %		
(mV)	Cd	Mg	S	
1445	29.97	9.97	60.13	
1450	36.35	11.21	52.44	
1455	39.16	13.29	47.59	
1460	39.40	15.52	45.08	

The EDS maps of ED CdS: Mg thin films produced at numerous deposition voltages are displayed in Figure 4.28. The analysis's findings verified that all of the targeted elements, including Cd, Mg, and S, were present on the map and that the deposition voltage changed their elemental composition. In addition, the carbon tape that was utilized to secure the sample to the SEM sample holder stud is the reason for the carbon peak. The CdS:Mg elemental composition with deposition

voltage is displayed in Table 4.5. According to the results of the analysis, the deposition voltage affected the proportion of CdS:Mg thin film components. Other signals from the ITO glass substrate, including In, Si, O, and Sn, were also identified. In the deposition voltages of 1445, 1450, 1455, and 1460 mV, respectively, the magnesium content rose and was measured at 10%, 11%, 13%, and 16%. As S decreases with deposition voltage, the Cd % also rises. At a deposition voltage of 11450 mV, the deposited film with a nearly stoichiometric composition of Cd, Mg, and S is measured. According to this study, the optimal deposition voltage for CdS: Mg thin film formation in the TEED technique in potentiostatic mode is 1450 mV.

4.6. Properties of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ using Density Functional

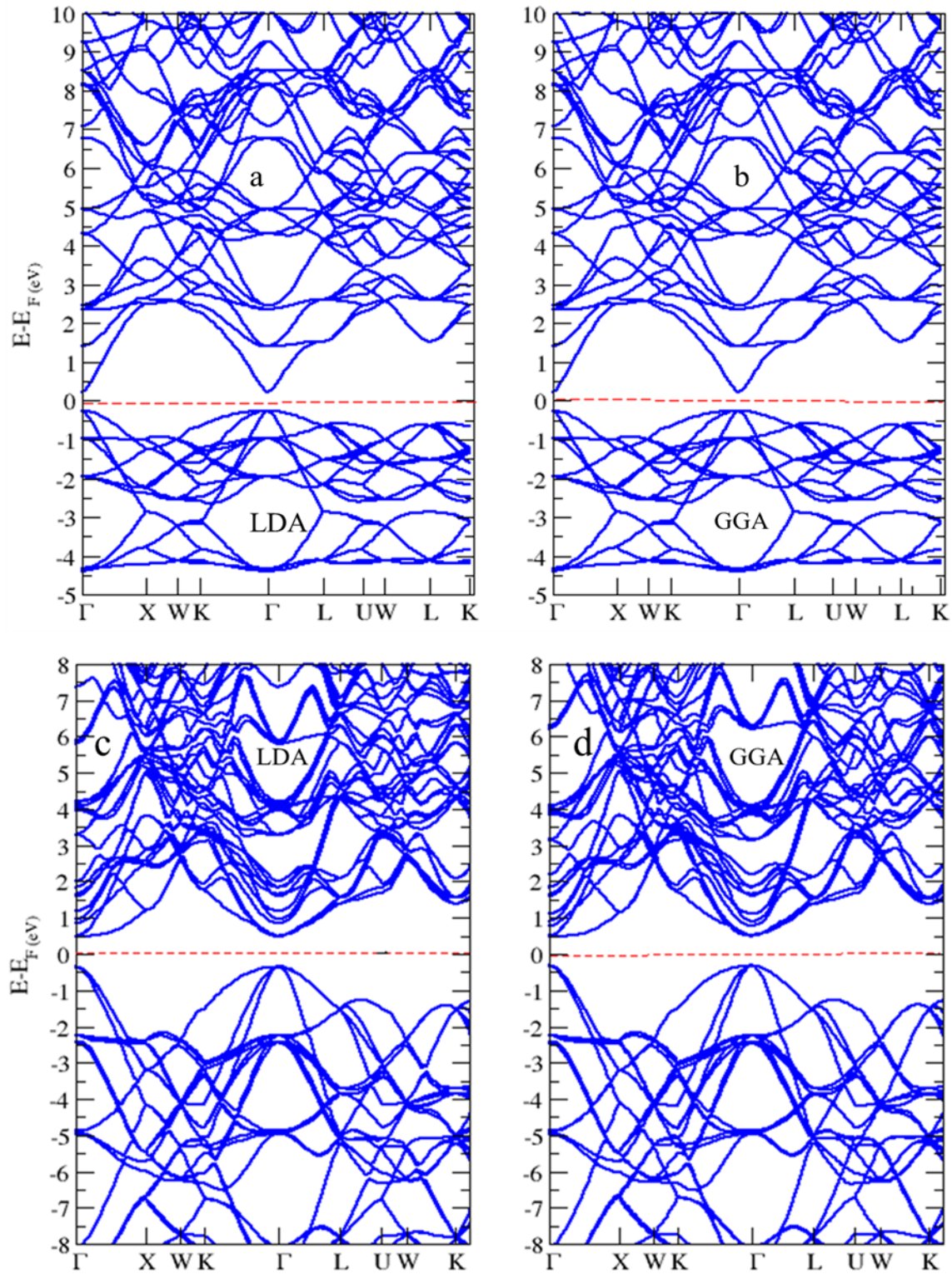
4.6.1. Band structure energy band gap

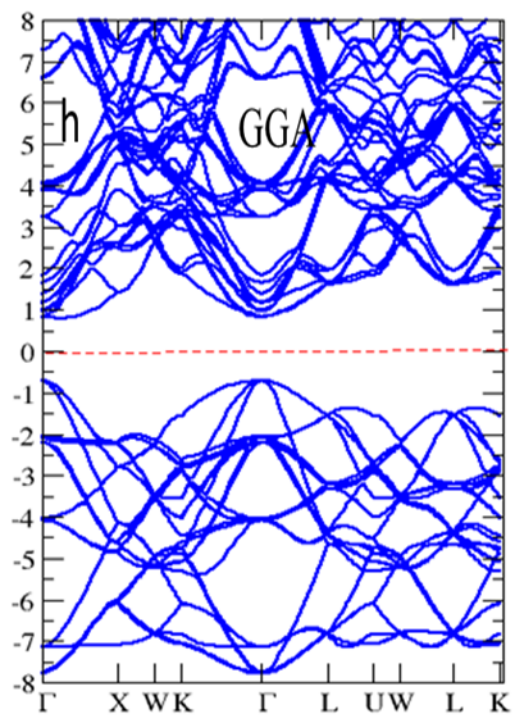
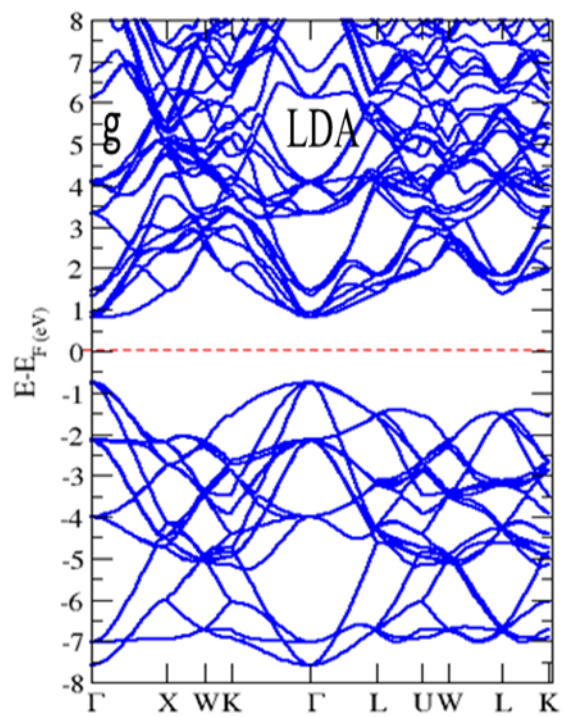
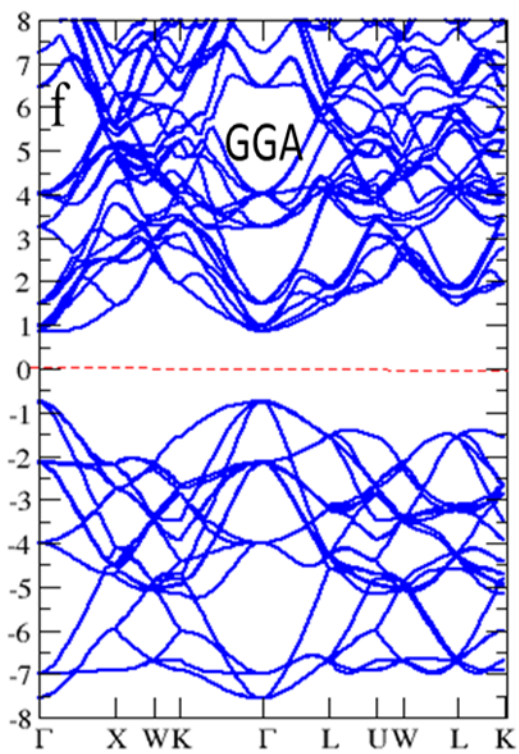
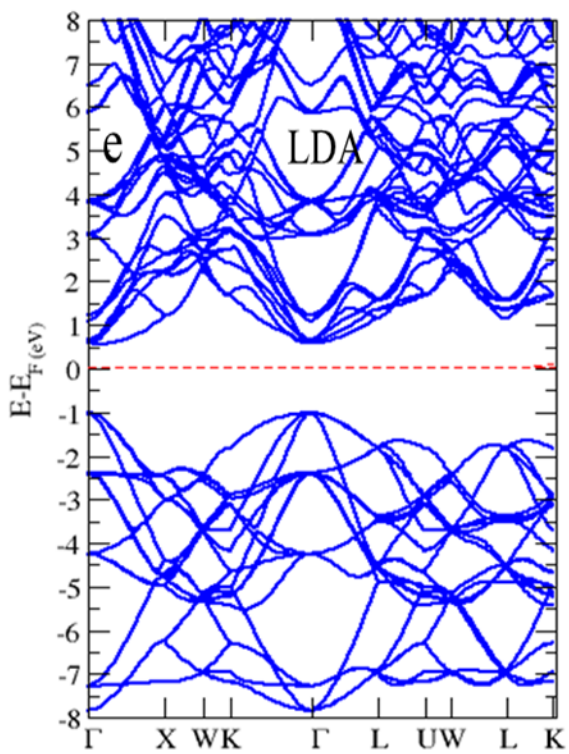
The band structure study plays a significant role in identifying whether the materials have a direct or indirect band structure. Finding the Fermi energy, which is necessary to occupy every level at zero temperature, is very significant. Depending on whether the Fermi energy is inside a band gap, a material can be either metallic or insulating.

The interactions between orbitals in the lattice determine compounds' energy band structure. For direct band-gap semiconductors, the valence band maximum (VBM) and conduction band minimum (CBM) for each occur at the same k-point, and for non-direct band gap was at different k-points. The computational investigations showed that compound semiconductors were calculated using a high symmetry point in the first Brillouin zone using both LDA and GGA approximations. In this study, as shown in Figure 4.29, it was observed that in both approximations of LDA and GGA, there is no significant difference in the band structure of CdTe and $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ but small values in band gap calculation. On the other hand, the band gap calculation was not the same as the experimental value (Yadav et al., 2021).

Figure 4.29 shows that energy structure for (a) CdTe -LDA and (b) CdTe-GGA, (c) $\text{Cd}_{0.75}\text{Zn}_{0.25}\text{Te}$ -LAD, (d) $\text{Cd}_{0.75}\text{Zn}_{0.25}\text{Te}$ - GGA, (e) $\text{Cd}_{0.05}\text{Zn}_{0.05}\text{Te}$ -LAD, (f) $\text{Cd}_{0.05}\text{Zn}_{0.05}\text{Te}$ -GGA, (g) $\text{Cd}_{0.25}\text{Zn}_{0.75}\text{Te}$ -LAD, (h) $\text{Cd}_{0.25}\text{Zn}_{0.75}\text{Te}$ -GGA, (i) ZnTe-LDA and (j) ZnTe-GGA. The calculated energy band gap of CdTe for LDA is 0.69 eV, and the energy band gap for LDA is 0.75 eV. Experiments show that the band gap of CdTe film varies from 1.45 eV to 1.48 eV(Narasimhan, 2015). This energy difference is due to weak exchange-correlation functional approximation for DFT since DFT is ground state charge density calculation with

different approximations. For the band gap calculations, as shown in Figure 4.29, the band gap of CdTe: Zn at various concentrations was calculated, as well as a and Cd_{1-x}Zn_xTe.





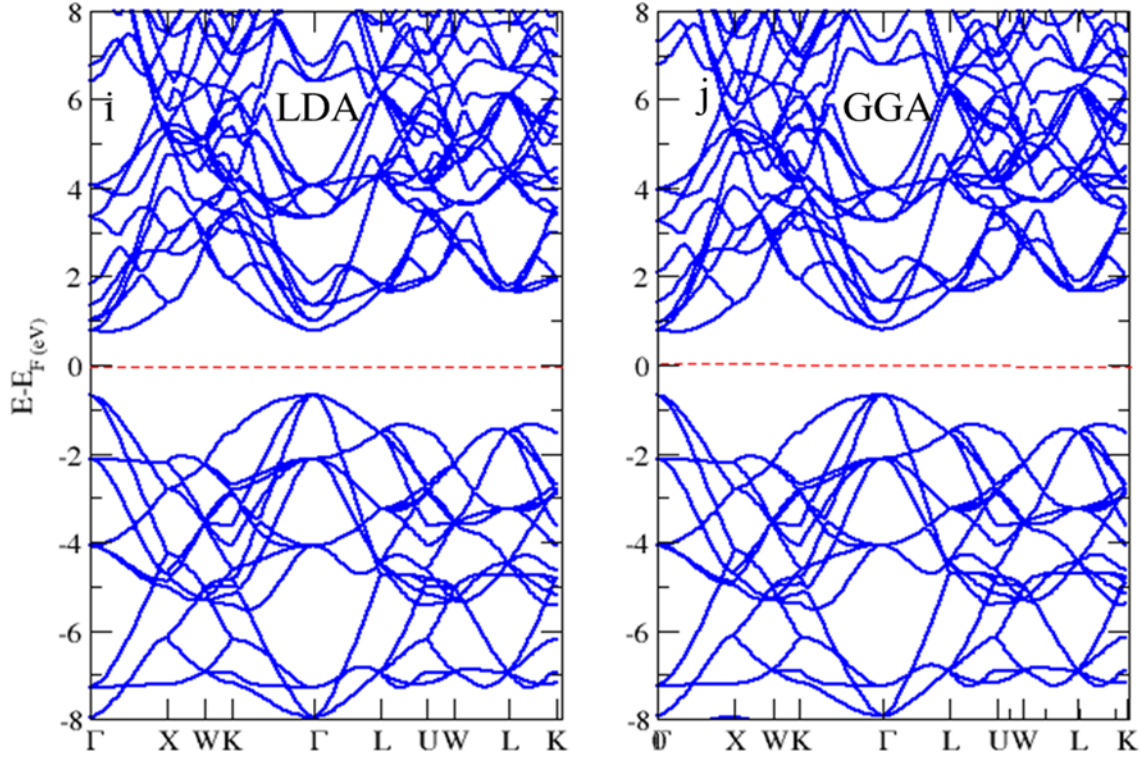


Figure 4. 29. The energy structure for (a) CdTe -LDA and (b) CdTe-GGA, (c) Cd_{0.75}Zn_{0.25}Te-LAD, (d) Cd_{0.75}Zn_{0.25}Te- GGA, (e) Cd_{0.5}Zn_{0.05}Te-LAD, (f) Cd_{0.5}Zn_{0.5}Te-GGA, (g) Cd_{0.25}Zn_{0.75}Te-LAD, (h) Cd_{0.25}Zn_{0.75}Te-GGA, (i) ZnTe-LDA and (j) ZnTe-GGA.

The energy band gap for Cd_{0.75}Zn_{0.25}Te, as shown in Figure 4.29 (c) and (d), was recorded as 1.02 eV and 1.15 eV for LDA and GGA, respectively. As the concentrations of Zn increased to Cd_{0.5}Zn_{0.5}Te, the energy band gap was increased and recorded as 1.60 and 1.64 eV with LDA and GGA approximations, respectively. Further, it increases to Cd_{0.25}Zn_{0.75}Te, and a slight increase in the band gap was observed, which is recorded as 1.62 and 1.69 eV for LDA and GGA approximation, respectively. For ZnTe, as shown in figure 4.29 (i) and (j), the bandgap was recorded as 1.71 and 1.76 eV with LDA and GGA, respectively. The overall band gap calculations show that it was less than the experimental results. One of the main challenges in band structure calculation is the energy band gap since density functional theory determines the ground state charge density calculation. To solve this problem, we use hybrid functional to include excited state electrons. Figure 4.29 Band structure and band gap Cd_{1-x}Zn_xTe with different concentrations of Zn (0.25, 0.5, and 0.75 %). In the whole range of values of the composition parameter (Zn content), the computed band structures demonstrate a direct bandgap for all three alloys with increasing order. The analysis results confirmed that CdTe has a direct band gap at Γ points, which agrees

with other reported and ED CdTe thin film experimental results (Yimamu, Afrassa, Dejene, Echendu, Terblans, et al., 2023a). The analysis of this result was in good agreement with our experimental results of ED of Cd_{1-x}Zn_xTe at different concentrations.

In these systems, the quadratic Vegard's law describes the link between band gaps and composition (Jin et al., 2024).

$$E_g(x) = E_{g1}(1 - x) + E_{g2}x + Ax(1 - x)$$

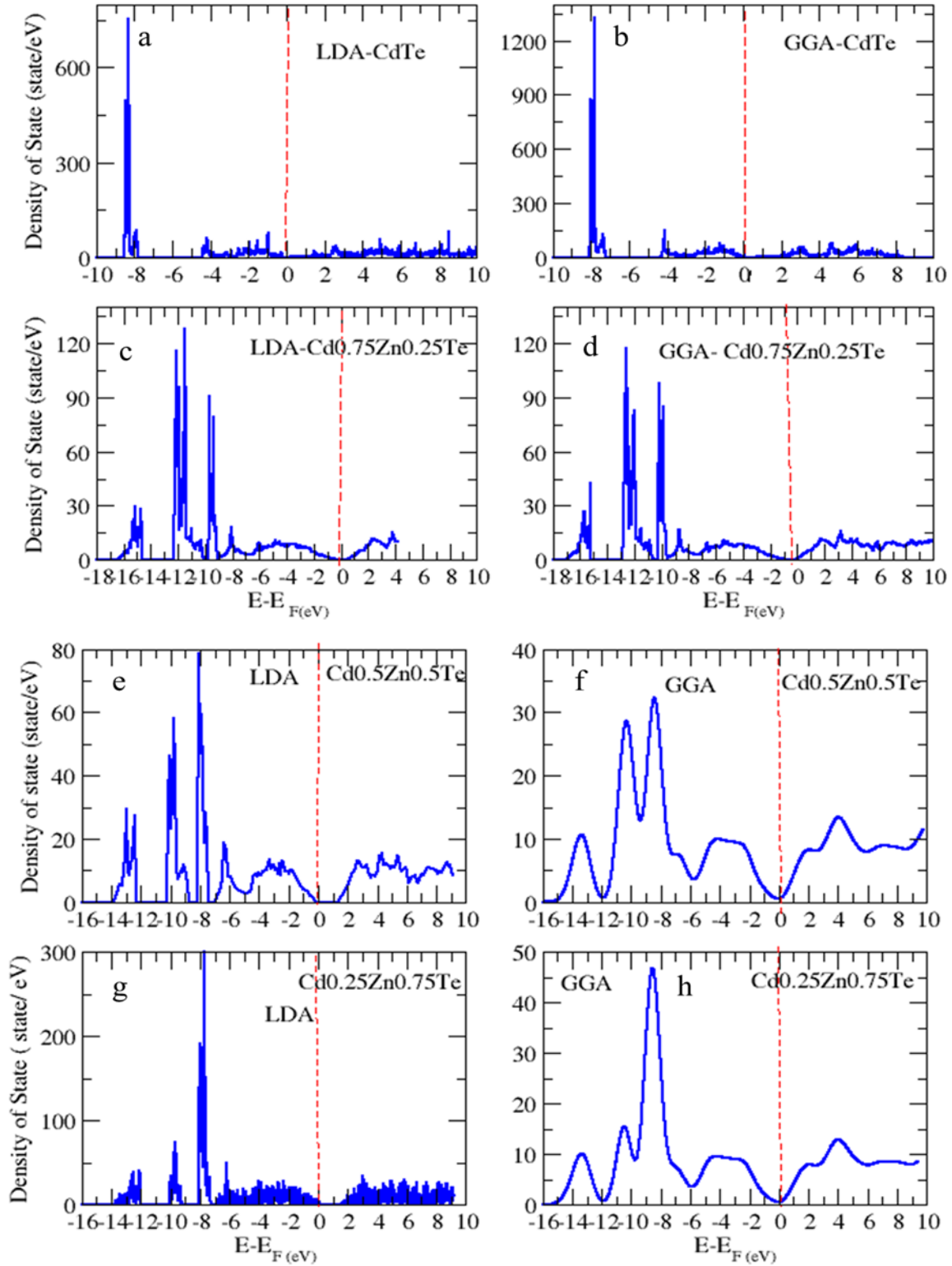
where $E_g(x)$ is the band gap energy as a function of composition x , and E_{g1} , and E_{g2} are the band gaps of the pure components. A is a coefficient that accounts for the non-linear contributions to the bandgap. For this case, CdTe and ZnTe are used as E_{g1} and E_{g2} with an energy band gap of 1.44 and 2.26 eV, respectively. The value of A is 0.1, which is taken from the literature. This model captures the curvature in the band gap versus composition plot, indicating that interactions between different atoms or ions in the alloy can lead to deviations from the linear prediction of Vegard's law. This is especially relevant in systems where electronic structure changes significantly with composition, such as in certain semiconductor alloys. The value is recorded as 1.66 eV, 1.87 eV, 2.07 eV, and 2.26 eV for 0.25, 0.5, 0.75, and 1 % Zn concentrations, respectively. From our experimental results, the energy band gap was varied with Zn-concentration recorded as 1.82, 2.02, 2.07, and 2.12 eV with 0.25, 0.50, 0.75, and 1.00 M Zn concentration, respectively.

4.6. 2 . The Density of State Calculation

The density of states (DOS) is computed using a simple histogram technique that needs many k-points mesh by the tetrahedron method [21]. (DOS) is the number of states that are available in a system, which is essential for determining the carrier concentrations and distribution energy of carriers within semiconductor materials. Figure 4.30 shows that the Density of state for (a) CdTe-LDA and (b) CdTe-GGA, (c) Cd_{0.75}Zn_{0.25}Te-LAD, (d) Cd_{0.75}Zn_{0.25}Te- GGA, (e) Cd_{0.5}Zn_{0.5}Te-LAD, (f) Cd_{0.5}Zn_{0.5}Te-GGA, (g) Cd_{0.25}Zn_{0.75}Te-LAD, (h) Cd_{0.25}Zn_{0.75}Te-GGA, (i) ZnTe-LDA and (j) ZnTe-GGA. In both approximations, LDA and GGA, the density of state and the level of fermi level varied with Zn-concentration.

Changes in DOS and the Fermi level shift may directly affect charge carrier recombination rates, which may alter the material's optical characteristics and carrier mobility. As Zn concentration rises from 0.25% to 1%, the DOS of Cd_{1-x}Zn_xTe changes. The conduction band undergoes

significant alterations, such as a shift in the bandgap, a broadening of conduction states, and the possible emergence of localized states.



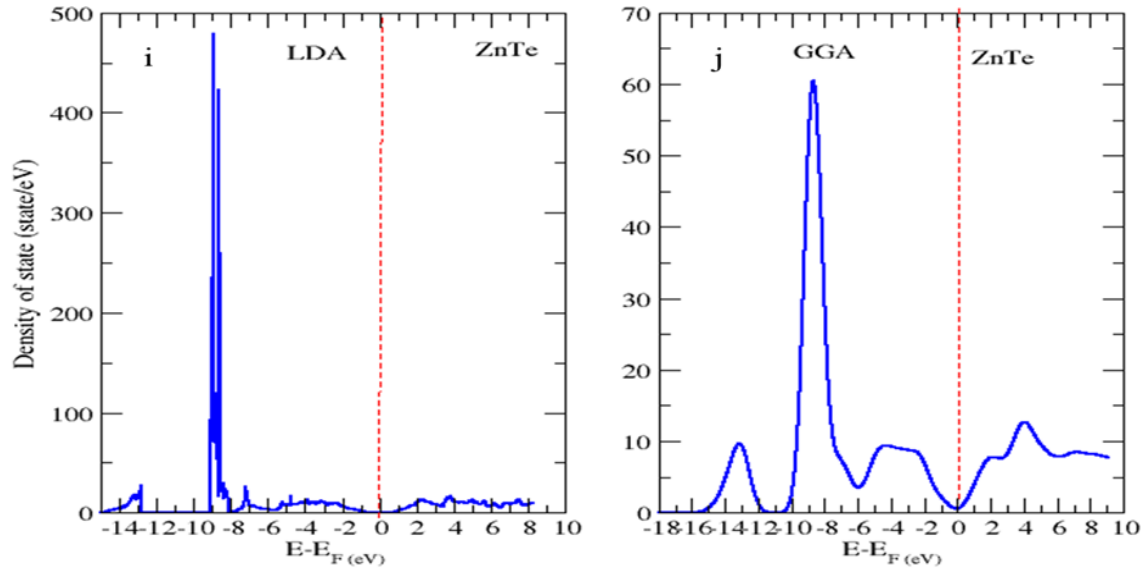


Figure 4.30 Density of state for (a) CdTe -LDA and (b) CdTe-GGA, (c) Cd_{0.75}Zn_{0.25}Te-LAD, (d) Cd_{0.75}Zn_{0.25}Te- GGA, (e) Cd_{0.5}Zn_{0.5}Te-LAD, (f) Cd_{0.5}Zn_{0.5}Te-GGA, (g) Cd_{0.25}Zn_{0.75}Te-LAD, (h) Cd_{0.25}Zn_{0.75}Te-GGA, (i) ZnTe-LDA and (j) ZnTe-GGA.

4.6.3. Lattice constant and Structure of CdTe

The lattice-constants calculation of CdTe has been determined using the PWSCF method with total energy by taking the number of lattice parameters around the current experimental value. As shown in figure 4.31 in quantum espresso PWSCF calculation of this study lattice-constant for CdTe by using GGA the value which is 6.508 Å, and the experimental lattice constant of CdTe was reported 6.501 Å and in zinc blend structure.

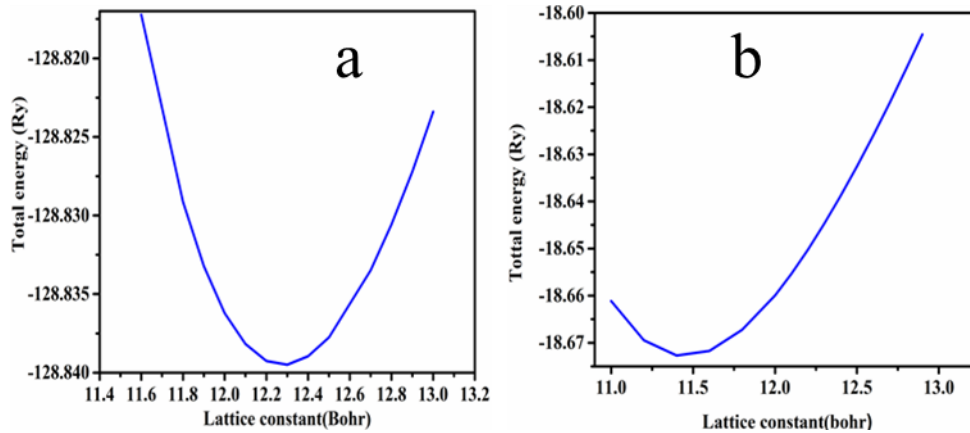


Figure 4.31. lattice constant vs energy for CdTe by using (a) GGA and (b) LDA

Our result shows that it is near the experimental lattice constant of CdTe. The lattice parameter CdTe calculated using LDA is far from the experimental value of CdTe. From this, we conclude

that GGA is a better approximation for lattice-constant determination than LDA. In lattice-constant calculation, another researcher can obtain the same result. ZnTe in the zinc-blend structure lattice parameter is underestimated by LDA and overestimated by GGA compared to the experimental (Bahloul et al., 2015). Visualization for Electronic and Structural Analysis (VESTA), a 3-dimensional visualization program for structural models, can be used to visualize the compound semiconductor CdTe in FCC zinc-blend structure. A space group is a self-consistent arrangement of symmetry elements in a crystal lattice. CdTe was found in the symmetry space_group_name_ H-M 261, which has a zinc blend structure.

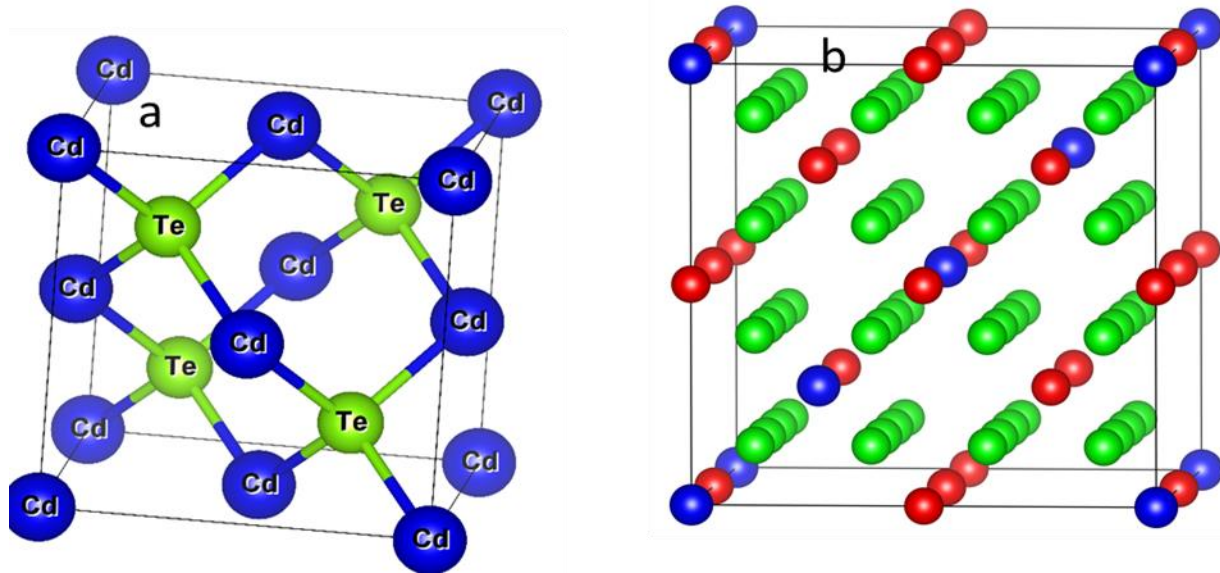


Figure 4. 3D visualization for (a) CdTe and (b) $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Te}$

4.6.4. Optical properties

Numerous techniques exist for calculating semiconductor dielectric constants; however, because of the tiny variations in unit cell size, the dielectric function is highly dependent on the electronic band construction of the crystal; the precision of these measurements has always been uncertain (Edossa & Woldemariam, 2020).

The kind of reaction that materials will display when photons are incident on them is determined by their optical characteristics, which include the imaginary component of the dielectric constant, the absorption coefficient, and an extinction coefficient. Analyses of the complex dielectric function can be used to estimate all optical properties (Iqbal et al., 2023). The polarization effects and dynamical screening strength are described by the real component of the dielectric function ϵ_1

(ω). Nonetheless, the energy absorption brought on by charge excitations is connected to the imaginary portion of the dielectric function $\epsilon_2(\omega)$ (Edossa & Woldemariam, 2020)

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega) \quad 4.1$$

optical parameters that offer information on the decrease in radiation speed as it travels through material and absorbs energy, such as the refractive index ($n(\omega)$) and extinction coefficient ($k(\omega)$), may also be calculated using the dielectric function. The following expressions can represent $n(\omega)$ and $k(\omega)$ numerically (Edossa & Woldemariam, 2020)

$$n(\omega) = \frac{1}{\sqrt{2}} \left[\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} + \epsilon_1(\omega) \right]^{1/2} \quad 4.2$$

$$K(\omega) = \frac{1}{\sqrt{2}} \left[\sqrt{\epsilon_1^2(\omega) + \epsilon_2^2(\omega)} - \epsilon_1(\omega) \right]^{1/2} \quad 4.3$$

Furthermore, the absorption coefficient may be used to calculate the material's optical absorption by utilizing the imaginary part of its refractive index. This coefficient also gives important information on how radiation decays with increasing distance. It may be shown mathematically in the following equation (4.4).

$$\alpha(\omega) = \frac{4\pi K(\omega)}{\lambda_o} \quad 4.4$$

It is possible to express reflection spectra in the following way, which is used to examine how incident light reacts to the material's surface by using equation (4.5).

$$R(\omega) = \frac{(n(\omega)-1)^2 + K^2(\omega)}{(n(\omega)+1)^2 + K^2(\omega)} \quad 4.5$$

The dielectric constant $\epsilon(\omega)$ calculations show that a smaller energy gap yields a larger static dielectric constant $\epsilon_1(0)$ [23]. The optical propriety of CdTe can be done by using post-processing code PWSCF and compiled by epsilon. From this, we get the real and imaginary parts of the material's dielectric constant. The result confirmed that when the imaginary part of the dielectric constant is the maximum point, the real part becomes the minimum, which is in good agreement with the reported results.

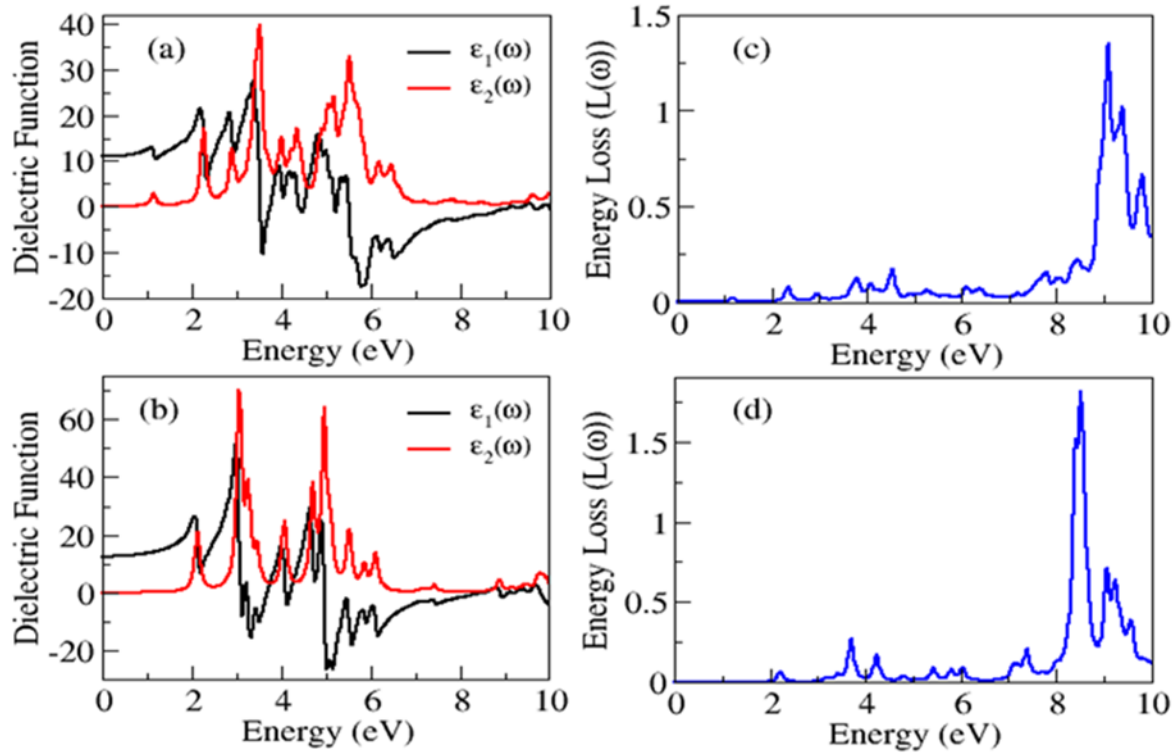


Figure 4. 33.The real and imaginary dielectric constant for (a) CdTe, (b) ZnTe, and Energy loss for (c) CdTe an (b) ZnTe.

The real and imaginary parts of the dielectric constant for CdTe varied with Zn concentrations. The first peak in CdTe was reduced when Zn- concentrations increased. Significant alterations in the dielectric characteristics occur when Zn is doped into CdTe (creating CdTe: Zn) for some reasons, including changes in the electronic structure, carrier concentration, and scattering processes. The observed shift in peaks for the real and imaginary components of the dielectric constant at various Zn concentrations may be explained in detail below. Zn is an impurity that is donated to CdTe. The electronic characteristics of CdTe are affected by the rise in free carrier concentration in the material, which coincides with an increase in Zn concentration. Carrier concentration and dielectric characteristics change when CdTe is doped with Zn, which adds more free charge carriers (electrons). Stronger screening of the Coulomb contacts results from a rise in the free carrier density, which influences the material's polarization and, consequently, the real component of the dielectric constant. Changes in the band gap or other aspects of the material's electrical structure, such as the Fermi level, can result from adding zinc. Both the real and imaginary components of the dielectric constant are impacted by these modifications, which alter

the material's optical absorption and responsiveness to electromagnetic fields (Abraham et al., 2015).

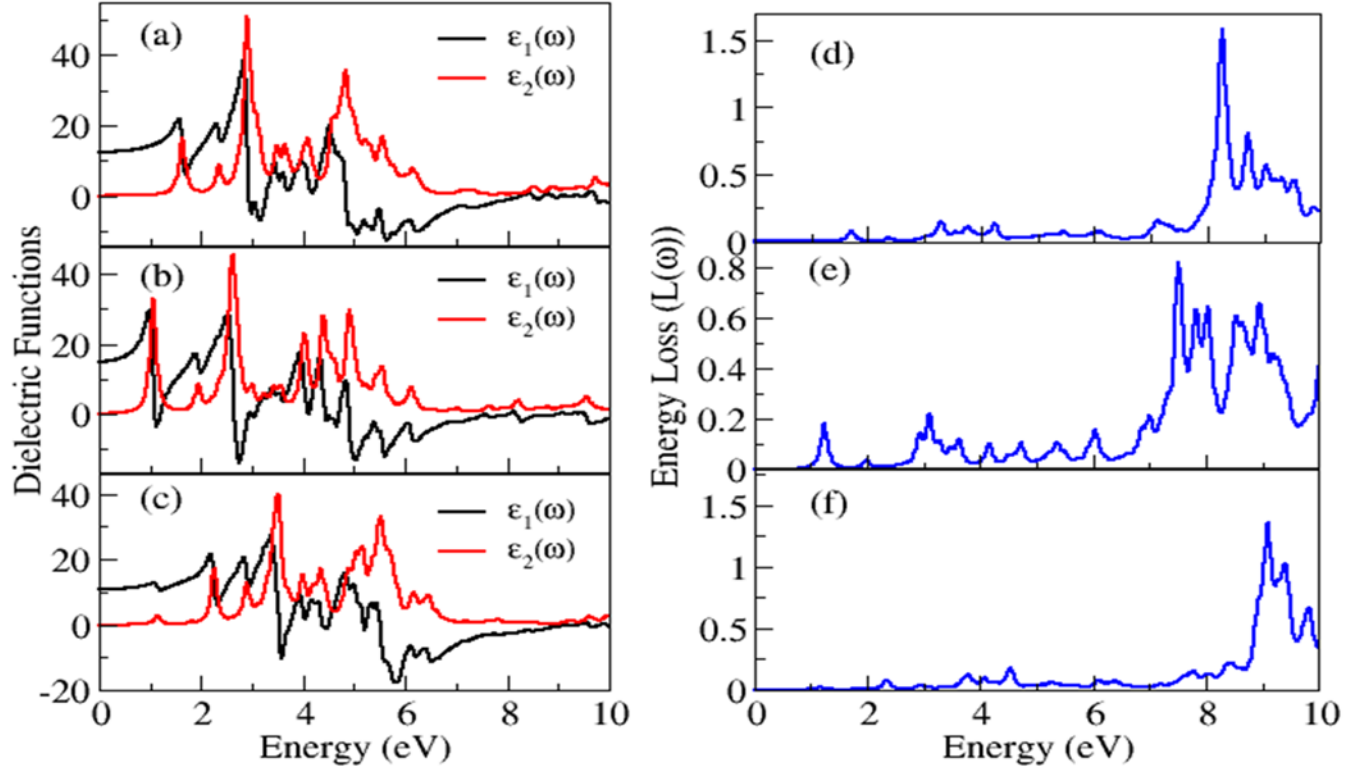


Figure 4. 34.The real and imaginary dielectric constant for Cd_{1-x}Zn_xTe with different concentrations of Zn (a) 0.25 (b) 0.5 (c) 0.75 % and Energy loss for different concentrations of Zn (d) 0.25 (e) 0.5 (f) 0.75 %

The change in carrier concentration, band structure alteration, and scattering effects brought about by Zn doping are the leading causes of the shift in peaks in both the real and imaginary sections of the dielectric constant for CdTe: Zn at varying Zn concentrations. These elements affect the material's dielectric response, energy dissipation, and polarization. The energy loss function as functions of photon energy was shifted towards the left when Zn-Concentrations were increased. As Zn concentrations in CdTe increase, the energy loss function (ELF) shifts to the right as a function of photon energy: Changes in carrier concentration, a rise in plasma frequency, improved screening effects, and maybe modified scattering processes are the main factors driving Zn. The observed shift in the ELF towards lower photon energies is caused by a reduction in the material's capacity to absorb and dissipate energy at higher photon energies as the Zn concentration rises.

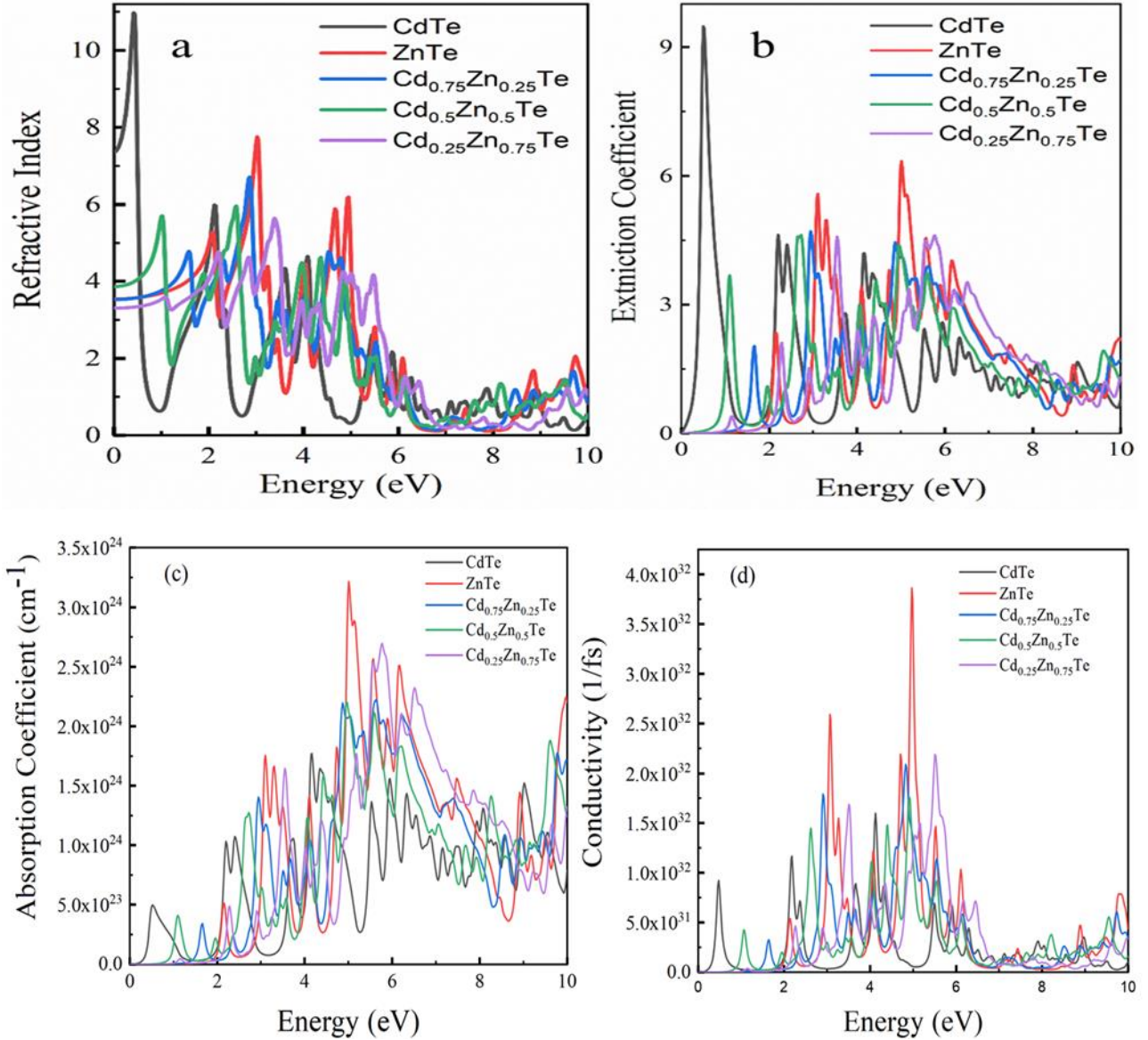


Figure 4.35. The properties of CdTe, Cd_{1-x}Zn_xTe, and ZnTe (a) refractive index, (b) extinction coefficient, (c) absorption coefficients, and (d) conductivity.

Refractive index (n) is a crucial optical characteristic that varies with temperature, doping concentration, and wavelength. Its dispersion properties make it very helpful in infrared applications, and the way it interacts with light is essential to the functionality and design of photovoltaic cells. Figure 4.35 (a) shows that the n value for CdTe: Zn at different Zn concentrations

The maximum peaks were observed at host CdTe at lower energy and varied with Zn - concentrations. The ZnTe had a maximum value of 3 eV and 5 eV. The unique feature was observed at Cd_{0.5}Zn_{0.5}Te, which may be due to the equal contribution of Cd and Zn for the study.

Light dissipation, caused by light scattering and absorption, usually happens when light travels through an elastic material. We refer to this occurrence as extinction. Extinction, to put it another way, is the degree to which a substance absorbs photons of a particular wavelength. The extinction of light is measured by the extinction coefficient (k). The dependences of the examined materials' extinction coefficients on photon energy are displayed in figure 4.35 b. The k values were varied with Zn- concentrations. The absorption coefficient and conductivity of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ varied with Zn- concentrations. The CdTe were dominated at a lower energy of less than 2 eV, and ZnTe was dominated at a higher energy of 5 eV; after that, it changed with different Zn concentrations. Figures 4.35 (c) and (d) show the absorption coefficient and Conductivity CdTe: Zn with Zn - concentration. The values of both absorption coefficient and conductivity vary with Zn concentration in a complex way, governed by the interplay of increased carrier concentration, changes in the band structure, and the introduction of defects and scattering centers.

5. Conclusions and Recommendations

5.1. Conclusion

ED of CdTe thin films was successfully grown on a conductive glass substrate (FTO) from an electrolytic bath solution containing cadmium acetate as Cd source and tellurium oxide as Te source. The XRD measurement confirmed that CdTe thin film varies with deposition voltage. It was a polycrystalline cubic zinc blend structure at (111) preferential orientation, and the best crystallinity was recorded at 1250 mV, crystallite size was 26 nm, and dislocation density and microstrain were calculated. UV-VIS analysis shows that the absorbance was varied with cathode potential, and the maximum was recorded at 1250 mV. The band gap calculation shows that CdTe thin films have 1.46 eV at 1250 mV deposition voltage near a band gap of 1.45 eV. PEC measurement shows that the thin film CdTe conductivity varied with voltage and p-type at low and n-type at high deposition voltage, which indicates that Te and Cd are rich thin films, respectively. This result agreed with previously reported results from different Cd sources.

Cadmium acetate was utilized as a Cd source, and CdTe thin films were successfully ED using two electrodes. The effects of pH on the structural, optical, surface, and compositional properties of CdTe thin films were examined, and the structural properties verified that the produced films have both cubic and hexagonal phases at pH values of 1.8, 2.5, and 3.5. At pH 3.0, a single-phase cubic structure was seen. The optical properties investigation demonstrates that the films' absorbance and energy band gap were impacted by deposition electrolyte pH in both the as-prepared and annealed samples, and the band gap values fluctuated as the deposition pH rose. SEM images show that the morphology, size, and shape of the CdTe thin layer grains changed with pH. According to the elemental composition analysis, the concentration of Te decreased while the content of Cd increased in CdTe thin films as the deposition pH increased. As the pH rose from 2.5 to 3.5, the Cd to Te ratio changed from 0.43 to 1.08 for the AD samples and from 0.92 to 1.32 for the HT samples. The ratio of Cd to Te was 0.88 for the as-deposited sample and 1.04 for the annealed sample at a pH of 3.0, indicating a nearly stoichiometric composition. SPM data showed that the average surface roughness of films changed with the electrolytic pH, reaching its maximum in both the AD and HT samples at pH 3.0. When the CdTe film is formed at a pH of 3.0, it may function as an absorber component in thin-film SC technology.

CdZnTe thin films were successfully made by using a low-cost TEED method with different concentrations of Zn. The study investigates the effect of Zn on the structure, optical, surface morphology, surface roughness, and elemental composition of CdZnTe. The structural analysis confirmed that the cubic structure CdZnTe was observed. The crystallite size, dislocation density, and microstrain of the films varied with Zn concentration. The optical properties of the films were increased with Zn concentration up to 0.5 M Zn and decreased from 0.75 to 1 M Zn. The band gap of CdZnTe was increased as Zn Concentration increased in both as-deposited and annealed samples. The surface morphology analysis showed that small grain agglomerated particles were observed for as-deposited samples, and some enhancement was observed after annealing. The average surface roughness properties were altered with Zn concentration. The maximum was recorded as 0.5 M Zn in both AD and HT samples. The compositional analysis confirmed that all the desired elements were detected in the films, and their composition varied with Zn-concentrations.

By employing a TE configuration and adjusting the deposition voltage, CdS: Mg thin film ED was successfully completed. The deposited samples were subjected to structural, optical, surface, and compositional studies. The polycrystalline structure of the CdS:Mg film was verified by the structural analysis, which also revealed a notable peak in the (110) plane.

The surface analysis verified that a CdS: Mg thin film covered the ITO glass substrate and that the shape of the film changed as the deposition voltage increased. As the deposition voltage increased, the R_q and R_a values changed as well; the lowest value was seen at 1450 mV. The longitudinal optic (1LO) phonon vibration of CdMgS was measured at wave numbers of 306 cm^{-1} , as validated by RS analysis. With observed wavenumbers of 486 cm^{-1} and 612 cm^{-1} , respectively, the second longitudinal optic (2LO) and the third longitudinal optic (3LO) are the two additional longitudinal optic phonons. All of the desired components were found in the films, according to compositional analysis, and their percentage changed with voltage. The film grown is more suited for possible window/buffer layer applications in SCs when the deposition voltage is 1450 mV. The remaining deposition parameters are intended to be improved for device formation in further studies.

The computational study using the first principle study by DFT implemented in the quantum espresso program, CdTe and $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ were successfully studied. The band structure, density of state, and dielectric properties of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ were calculated. The values in both LDA and GGA were estimated using an exchange-correlation approximation. The band gap CdTe was

increased as Zn concentrations were increased. The dielectric constant real and imaginary dielectric functions, reflective index, and absorption coefficients are changed with Zn-concentration.

5.2. Further Research and Recommendation

In fabricating CdTe thin films for SCs, achieving high-quality films is critical to ensuring optimal device performance. One of the most influential factors in the deposition process is the deposition voltage, which affects the thin films' morphology, composition, and structural properties. Based on my research recommendation, optimizing the deposition voltage with a small interval of 1 mV aims to enhance the quality of the films and improve the overall device performance. The recommendation to optimize the deposition voltage with a 1 mV interval suggests that small voltage adjustments can significantly impact the final film properties. By carefully monitoring these small changes, researchers can fine-tune the films to achieve better morphology, composition, and quality, directly translating into improved SC performance.

The proposed combination of CdS:Mg as the window layer and CdTe:Zn as the absorber layer presents a promising alternative to the conventional CdS/CdTe structure. By improving carrier mobility, junction quality, and stability, this new structure offers the potential for more efficient and durable thin-film SCs. Therefore, we recommend fabricating CdTe-based SCs using the CdS:Mg/CdTe:Zn combination for enhanced performance and stability.

List of Publications

1. **A. U. Yimamu**, M. A. Afrassa, F. B. Dejene, O. K. Echendu, J. J. Terblans, and H. C. Swart, “The effect of electrolytic solution pH on the properties of ED CdTe thin films for SE application, journals of *Optical Materials*. <https://doi.org/10.1016/j.optmat.2024.115340>
2. **A.U. Yimamu** , S.Z. Werta , F.T. Maremi , B.F. Dejene , O.K. Echendu: Effect of deposition voltage on the physico-chemical properties of ED Mg-doped CdS thin films for Opto-electronic application, 2024 *Materials Today Communications*: <https://doi.org/10.1016/j.mtcomm.2024.111410> .
3. **Yimamu, Ahmed Umer**, Fekadu Tolessa Maremi, Solomon Zerihun Werta, Francis Birhanu Dejene, Ibrahim Mohammed Beker, Vanthini Nelson Adoons, Megersa Kassim Hussen, Selepe Joel Motloun, and Jacobus J Terblans.. “Effect of Cathodic Voltage on Structural , Optical , and Surface Properties of ED of CdZnTe Thin Film for Optoelectronic Applications 2024 ASTU Ethiopian Journal of Science and Sustainable Development DOI: <https://doi.org/10.20372/ejssdastu:v12.i1.2025.980>
4. First Principal Calculation for CdTe and $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ Comparative Study for SE Applications: **submitted to journals of electronic structure**
5. Investigation of the effect of Zn Concentration on the Structural, Optical, and Surface Properties of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ Thin Films for Potential SC Applications. Submitted to journals of optical Materials. **Ready to submission**
6. **A U Yimamu**, M A Afrassa, F. B. Dejene, K.G. Tshabalala, S Z Werta, J J Terblans, H. C. Swart, Selepe Motloun, The effect of growth voltage on the structure, electrical and optical properties of CdTe thin films prepared by ED method, Harla J. Appl. Sci. Mater. 2022 1(1): 46-56, Harla Journals

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