1.1. Introduction

One of the most critical challenges facing countries across the globe is harnessing energy from renewable sources in an efficient, cost-effective and sustainable manner. The reckless exploitation of fossil fuel resources has caused serious imbalances in the biodiversity and has begun to pose a serious threat to quality of life in the earth. In the search for a perennial source of safe, clean and sustainable energy, energy managers and experts throughout the globe now unanimously agree that tapping the inexhaustible and bountiful solar energy offers the best hope for mankind.

It has been estimated that sunlight provides by far the largest of all carbon-neutral energy sources and that more energy from sunlight strikes the earth in one hour than all energy consumed on the planet in a year. The solar resource is presently exploited in a miniscule fraction of its potential through solar electricity which is a $7.5 billion industry growing at a rate of 35-40% per annum. Solar electricity currently provides only approximately one-millionth of the total electricity supply, and renewable biomass provides less than 0.1% of the total energy consumed. The huge gap between the present use of solar energy and its enormous undeveloped potential presents a great challenge to energy researchers.

Solar technology has been stuck for decades, with only minor incremental improvements in silicon-based cells, never achieving more than 30% efficiency ratios for converting sunlight to electricity. However, this malaise in solar technology appears to be coming to an end, due to advancements in nanotechnology -building structures on the molecular level and with phenomenal advances in thin film technologies.

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Photovoltaic conversion of solar energy is one of the most promising ways of meeting the increasing energy demands of the future in a time when conventional sources of energy are being exhausted. Photovoltaic conversion has many advantages over conventional energy conversion. Electricity produced from photovoltaics has a far smaller impact on the environment than traditional methods. Conventional methods (e.g. burning coal, petroleum and other fossil fuels, and waste incineration plants) produce pollutants such as carbon dioxide, carbon monoxide, and others. These pollutants are responsible for the greenhouse effect and global warming [1]. Furthermore, fossil fuels and uranium (nuclear energy) are non-renewable resources. The only resource needed to power a solar cell is sunlight. Since the sunlight is clean, abundant and virtually limitless, solar cells are non-polluting and a renewable alternative to conventional energy sources. As solar cells have a useful life in excess of twenty years, they can be considered as long-life devices [2]. Capturing solar energy typically requires equipment with a relatively high initial cost. However, over the lifetime of the solar equipment, these systems can prove to be cost-competitive, as compared to conventional energy technologies. The key to successful solar energy installation is to use quality components that have long lifetimes and require minimal maintenance. This is the motivation factor to carry out the research on a photovoltaic material for the solar cell applications.

1.2. Solar cell materials

The conversion efficiency and performance of a solar cell depend on its material properties, design and fabrication process. The major strategy to make PV energy more economical focuses on cheaper materials and manufacturing techniques. Instead of single-crystal materials, a number of polycrystalline thin-film technologies have emerged as promising candidates for PV energy conversion. Potential semiconductor materials used in solar cells are single crystalline silicon (Si), amorphous Si and polycrystalline thin films. Among

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polycrystalline thin films copper-indium-diselenide (CuInSe₂) and cadmium-telluride (CdTe) are the most popular. Discovering the properties and the potential of the CdTe thin film solar cell is the topic of this thesis. The objective of this thesis is to study the CdTe thin film layers and the CdTe/CdS solar cells. This study has been carried out in order to improve the understanding of thin film CdTe solar cells and to develop improved processing schemes. The figure 1.1 shows the status of the various solar cell materials and their achieved efficiencies. From the figure it is shown that in the hetero junction solar cells Cadmium Telluride is showing the highest optimal efficiencies.

**Figure 1.1:** Status of the Solar cell efficiencies of various solar cell materials.

### 1.3. Significance of the CdTe Material

CdTe is an excellent choice for use as a semiconductor in solar panels because it is best matched to the solar spectrum. Due to the optimum band gap of
1.5 eV as shown in figure 1.2 and high optical absorption at the band edge, the CdTe has a special status among the photovoltaic materials. Cadmium sulfide provides semiconductor properties, and its transparency allows the sunlight to pass through to the CdTe layer. These characteristics provide the potential for high-efficiency modules with low-cost manufacturing processes. A CdTe PV module contains very little cadmium. In fact, it has less than 0.1% cadmium by weight. One 8-square-foot module contains less cadmium than one size-C NiCd flashlight battery, and the cadmium in the module is in a much more environmentally stable form (i.e., a compound rather than a metal). Because cadmium is encapsulated in the PV module, PV technology provides an effective solution for sequestering cadmium. PV modules seal the cadmium for the life of the module (20-30 years), at which time the cadmium can be easily recycled. PV modules use natural elements and compounds to generate clean, emissions-free energy. Consumers face much greater hazards from the use of conventional energy, which can produce acid rain, particulates, noxious fumes, carbon dioxide, and small amounts of heavy metals. PV modules produce no pollutants during operation, making them the perfect solution for offsetting emissions (including cadmium) that result from fossil fuel use. The potential for cadmium use in the solar energy industry to ameliorate global climate change cannot be ignored. In the future, using a relatively small amount of cadmium for PV (about 2,000 metric tons per year) could change the world's electricity infrastructure; in comparison, the much larger, existing use of cadmium for other applications (about 20,000 metric tons per year) provides trivial value. The figure 1.2 shows the band gap of the various semiconductor materials and the CdTe shows the optimum band gap and maximum efficiency.
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Figure 1.2: Achieved Efficiency of the various solar cells with their band gap.

1.4. Zinc Blende structure of CdTe

Figure 1.3: Zinc blende structure of the Cadmium Telluride
The diamond, zinc blende and wurtzite structures are the three most common crystal structures of semiconductors grown for practical applications. The diamond structure consists of two interpenetrating face-centered-cubic (fcc) sublattices displaced from each other by \((1/4, 1/4, 1/4) \) \(a\), where ‘\(a\)’ is the cube edge length, often called the lattice constant. The zinc blende structure also has the same sublattices, except that the anions occupy one sublattice, while the cations sit on the other. Both structures have an fcc lattice with two atoms per unit cell. Figure shows the arrangement of the atoms inside a cube of the zinc blende structure. The zinc blende structure can be described most easily by examining the stacking sequence of planes of close-packed spheres of the same radius along the \((111)\) direction.

The zinc blende structure consists of fcc lattice. Associated with every lattice site there are two atoms which are displaced relative to each other by one quarter of the body diagonal along \((111)\) direction. The volume defined by the primitive lattice vectors and containing these two atoms forms a unit, known as the primitive cell, which is repeated at each lattice site. One simple way to construct these crystal structures is to start with two fcc sublattices, each containing only one atom located on every lattice site. Then one sublattice is displaced by one quarter of the body diagonal along the \((111)\) direction with respect to the remaining sublattice. In the resulting crystal structure four nearest neighbors forming a tetrahedron surround each atom. The zinc blende structure with lattice parameter \(a = 6.481\text{Å}\) is the stable form for bulk single crystals of CdTe at atmospheric pressure. Zinc blende structure of CdTe is most preferable choice for the solar cell device applications.

1.5 CdTe/CdS Solar Cells

CdTe has emerged as a promising thin film material for a number of reasons. Its 1.5 eV band gap is quite ideal for terrestrial energy conversion [3].
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CdTe also has a very high absorption coefficient, meaning that relatively thin layers can be used to make effective functional devices. Finally, CdTe films are amenable to a variety of synthesis techniques, as detailed below. One potential problem with CdTe technology is that cadmium is a heavy metal. As such, there are concerns that the deployment of large quantities of CdTe solar cells could result in cadmium pollution of the environment. This is an issue that has been thoroughly studied and not thought to be a showstopper. The real time efficiencies [4 -12] of these cells are lower than the predicted efficiencies. So, much work is required to optimize the materials as well as the fabrication techniques. Due to the optimum band gap and high optical absorption at the band edge, the CdTe has a special status among the photovoltaic materials. By the end of 1970s the reported efficiencies of CdTe based (single crystal) solar cell devices were about 8%. The work on CdTe thin films got much attention in the 1980s with the development of various techniques such as electro deposition, screen printing, thermal evaporation and close spaced sublimation (CSS) and efficiencies of about 13% was achieved for CdS/CdTe hetero-junction solar cells.

Among the various techniques for depositing thin films of CdTe, the most successful method is the close spaced sublimation. The present status of thin film CdTe based solar cell is about 16% efficiency for devices on glass substrates [4] and 5.3% efficiency for devices on metallic substrates [13] all prepared by CSS. The work on metallic substrate based devices has received much attention only recently and the efficiency is expected to increase further with the possibility of exceeding that of glass based devices. But the predicted theoretical efficiency of 24% [14] is still far away posing a challenge to the photovoltaic researchers. Substantial increases in cell efficiency can only be obtained by an improvement of the CdTe/CdS junction. Like all hetero junctions, CdTe/CdS has defects at the metallurgical junction due to lattice mismatch, thermal expansion mismatch, and differences in the electron affinities of the two materials. In addition there will
be non-stoichiometric surface layers on the film surface. All of this adversely affect either the $V_{oc}$ or the Fill Factor or both and are obstacles to greater efficiency. The goal of this thesis, therefore, is to raise the efficiency of CdTe/CdS cells by improving the junction and accordingly raising open circuit voltage and Fill Factor.

Cadmium telluride has been used to make photovoltaic devices for quite some time. Many different CdTe devices have been fabricated in a number of different configurations. CdTe is a semiconductor that can be made both p-type and n-type [15]. This property led early researchers to investigate all-CdTe homojunction cells [16]. This work eventually led to 10.7% efficient devices of this type [17]. Studies of CdTe heterojunctions were also undertaken. Early efforts focused on n-type CdTe combined with various p-type materials. In the early 1960s, Cusano fabricated 6% devices by depositing thin p-Cu$_{2-x}$Te films on n-CdTe substrates [18]. However, these devices were not stable, and the overall lack of suitable p-type layers led to a different approach for making heterojunction CdTe cells. Work on CdTe heterojunctions began to focus on the use of p-type CdTe. Adirovich et al reported the first thin-film device of this type in 1969 [19]. The cell consisted of a CdTe thin film evaporated onto a CdS/SnO$_2$/glass superstrate. The conversion efficiency of this first cell was only 1%, but this device structure would prove to be very promising. Within ten years, Bonnet and Rabenhorst had made CdTe/CdS heterojunctions by evaporating CdTe films onto Mo foils [20]. Their success fueled further interest in CdTe/CdS technology. By 1982, Kodak researchers Tyan and Perez-Albuerne had produced the first 10% efficiency cell [21]. Subsequent refinement of the same superstrate structure first demonstrated by Adirovich et al has culminated with record device efficiencies of over 16% [4,22,23]. The CdTe is one of the most studied materials for its suitability upon solar cells [24-56]. However there is only a limited systematic study on the CdTe layer processing for the solar cell applications.
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This thesis focuses its study on vacuum evaporated CdTe thin films and the role of post deposition treatments and film thickness in a systematic manner.

1.6. Objectives

The purpose of this thesis is to increase the fundamental understanding of CdTe thin films and CdTe based solar cells. The systematic study of the properties of the CdTe layers reveals information about how future improvements to solar cells may be made. Understanding the CdTe absorber layer electronic properties and how they change due to the application of processing steps is the main objective of this thesis. The combination of routine as well as novel characterization techniques were used to characterize these films. These properties were observed under various processing conditions. The main objective of this thesis is to study the properties and their dependence on film thickness, post deposition treatments i.e. annealing and CdCl₂ treatment of vacuum evaporated CdTe thin films. Moreover, in the present work, an attempt has been made to study the electronic band structure for the CdTe thin film of zinc-blende type structure using the experimentally calculated results within the density functional theory (DFT) in the local density approximation (LDA).

1.7 Outline

The organization of the thesis have been outlined as follows

Chapter II  The experimental and analytical techniques used to prepare and characterize the Cadmium Telluride (CdTe) thin films have been dealt in this chapter.

Chapter III  Structural and surface characterizations of the CdTe thin films prepared by vacuum evaporation technique. The dependence of the structure of the CdTe thin films with film thickness, annealing and CdCl₂ treatments has also been discussed elaborately in this chapter. Scanning Electron Microscopy
(SEM) and Atomic Force Microscopy (AFM) techniques have been used to analyze the surface of the Cadmium Telluride (CdTe) thin films and their results have been also given in this chapter.

**Chapter IV** The optical transmittance and absorption spectra were recorded to study the optical properties like optical transition, optical band gap, optical constants etc. and their dependence on film thickness and post deposition treatments is discussed.

**Chapter V** The electronic structural characterization of the CdTe thin films by *ab-initio* calculations using the experimentally calculated lattice parameter values.

**Chapter VI** Dielectric and electrical conduction studies on the Metal/CdTe/Metal (MSM) devices have been given in the chapter. The electrical conduction mechanisms in the CdTe films have been studied under AC and DC fields and the results are also discussed in the chapter.

**Chapter VII** The photoconduction properties of the CdTe films have been analyzed and the results are given in the chapter.

**Chapter VIII** Solar cells with the structure ITO/ p-CdTe -n-CdS/Ag has been fabricated and the cell characteristics have been discussed in the chapter.

**Chapter IX** Summary and important conclusions of thesis have been given in the chapter.
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