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# ASSESSING THE PROPERTIES AND APPLICATIONS OF TITANIUM DIOXIDE (TIO2)

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## ABSTRACT

Due to their high-quality physical, optical, and electric features, metal oxide thin films have achieved remarkable success in the semiconductor industry. Solar cells, biosensors, biomedical applications, super capacitors, photo catalysis, luminous materials, and laser devices are only some of the potential applications for these materials, which are gaining increasing attention. Many studies have reported successful attempts at producing thin films using a wide variety of deposition techniques. Films' qualities need to be characterized in detail so that their design may be optimized. Thin-film solar cells, perovskite solar cells, and dye-sensitized solar cells are the primary research and development foci in this study. Solar cells made under varying circumstances were analyzed for their photovoltaic properties (short-circuit current, open-circuit voltage, fill factor, and efficiency). The experimental results verified the feasibility of using metal oxide as an electron transport layer, electron conducting medium, anti-reflection layer, and whole transport material.

**Keywords: -** Material, Dioxide, Surface, Circuit.

## I. INTRODUCTION

Surface engineering involves changing the properties of the surface and near- surface region in a desirable way. Surface engineering can involve an overlay process or a surface modification process. Each process has its advantages, disadvantages and applications. In some cases surface modification processes can be used to modify the substrate surface prior to depositing a film or coating. For example a steel surface can be hardened by plasma nitriding (ion nitriding) prior to the deposition of a hard coating by a PVD process. In other cases, a surface modification process can be used to change the properties of an overlay coating.

An atomistic film deposition process is one in which the overlay material is deposited atom-by-atom. The resulting film can range from single crystal to amorphous, fully dense to less than fully dense, pure to impure, and thin to thick. Generally the term “thin film” is applied to layers which have thicknesses on the order of several microns or less (1 micron = 10-6 meters) and may be as thin as a few atomic layers. Often the properties of thin films are affected by the properties of the underlying material (substrate) and can vary through the thickness of the film. Thicker layers are generally called coatings. Atomistic deposition process can be done in vacuum, plasma, gaseous, or electrolytic environment.

One of the principal characteristics of materials is their ability to conduct electrical current. Indeed, materials are classified by this property that is, they are divided into conductors, semiconductors and insulators or dielectrics. Conductors are characterized by partially filled valence bands and that the electrons in these bands give rise to electrical conduction. On the other hand, the valence bands of insulators are completely filled with electrons. Semiconductors, finally represent in some respect a position between conductors and insulators.

## II. MATERIALS PROPERTIES OF TITANIUM DIOXIDE (TIO2)

TiO2 material is a versatile one which is finding application in many scientific devices. It is highly useful in developing solar cells and also in the field of gas sensors. So, its materials properties are summarized here.

**Glypses of TiO2**

The physical, optical, electrical and chemical properties of titanium dioxide (TiO2) depend greatly on the amorphous or crystalline phase of the material. TiO2 is complex material with three crystalline phases, two of which are commonly observed in thin films – anatase and rutile and the brookite phase is uncommon. All three of these types are expressed using the same chemical formula (TiO2); however, their crystal structures are different.

Anatase is commonly observed at film deposition temperatures of 350-700 oC, while higher temperature promotes the growth of rutile. The third phase brookite has an orthorhombic crystalline structure and it is an unstable phase and it is of low interest. Deposition temperatures lower than 300oC generally result in the formation of amorphous TiO2.

The most common form is rutile which is also the most stable form. Anatase and brookite both convert to rutile upon heating. Rutile, anatase and brookite all contain six coordinate titanium. Additionally, there are three metastable forms produced synthetically and five other forms on applying high pressure.

Since TiO2 exists in several phases, it has different optical, electrical and chemical properties and therefore extensive literature review has to be performed to understand how the TiO2 films would behave in different processing conditions. This chapter will therefore describe the properties of the crystalline phases most commonly observed in thin films, that of rutile, anatase and amorphous TiO2. The third crystalline phase, brookite is a less stable and common form of TiO2 is rarely observed in deposited thin films and will not be discussed here. There are many different parameters that affect the phase of a deposited TiO2 thin film. Some of these parameters are deposition method, deposition temperature, annealing temperature, deposition rate, deposition pressure, precursor type, reaction atmosphere, impurities present and substrate type. The resulting phase or mixture of phases plays a role in determining the physical, optical, chemical and electrical properties of the film. A summary of all these properties are presented in the following sections of this chapter.

## III. APPLICATION OF TIO2

TiO2 thin films are useful for number of optical coatings, waveguides, optoelectronic, electrochromic devices, integrated circuits and in paint industry. Most of these applications are consequence of its micro or nano-structured TiO2 powders/thin films.

Therefore it is better to know the application fields before going for the preparation of high quality semiconducting TiO2 thin films. Some of the applications are summarized below.

i. The room-temperature ferromagnetism (RTF) behavior was confirmed in the co- doped TiO2 thin films. By processing metal-ferromagnetic-semiconductor heterostructures, the speed of data processing and larger charge storage capacity can be increased. The RFT technology is now used in information technology and spintronics [88].

ii. Dye-sensitized solar cells (DSSCs) have been the subject of intense study on account of their high conversion efficiency and low cost. Transparent and conductive TiO2 is a suitable material for the fabrication of such solar cells [89].

iii. Titanium oxide absorbs light having an energy level higher than that of the band gap, and causes electrons to jump to the conduction band to create positive holes in the valence band. Despite, the fact that the band gap value is 3.0 eV for the rutile type and 3.2 eV for the anatase type, they both absorb only ultraviolet rays. However, the rutile type can absorb the rays that are slightly closer to visible-light rays. As the rutile type can absorb light of a wider range, it seems logical to assume that the rutile type is more suitable for use as a photocatalyst [35].

iv. In titanium oxide, the absorption of ultraviolet rays with a wavelength of 388 nm or shorter promotes reactions; however, it is known that 254 nm rays having a greater energy level, which are used in germicidal lamps, are absorbed by the DNA of living organisms and form pyrimidine dimers, thereby damaging the DNA [35].

v. When photocatalytic TiO2 is irradiated by UV light, it produces pairs of electrons and holes. The created holes in valence band generated hydroxyl radicals, and the excited electrons in the conduction band generated superoxide anions, those strong oxidative radicals can decompose organic compounds as TiO2 photocatalyst effect. In 1985, Matunaga et al [90] reported for the first time the microbiocidal effect of TiO2. Since then, research works on photocatalytic killing has been intensively conducted on a wide variety of organisms including viruses, bacteria, fungi, algae, and cancer cells [91].

vi. TiO2 has been applied to a variety of environmental problems especially in water and air purification. Although TiO2 powder has been widely used, the difficulty of recovering the powder from treated water is a major obstacle. In many studies, some research groups have immobilized TiO2 films onto supports to avoid further separation process [92].

vii. TiO2 films have attracted much attention for optical, electrical and environmental applications [93, 94] because of their high refractive index and dielectric constant. TiO2 films can also be used as optical materials, such as antireflective coatings, high- reflectance films and wavelength-selective films [95], electronic materials such as insulator films of capacitors.

viii. The photons with energies greater than the band gap are absorbed by TiO2 and electron–hole pairs are generated. The holes photogenerated in TiO2 have strong oxidizing power and organic compounds can be completely decomposed to CO2, H2O, etc. [96, 97].

ix. Due to the high refractive index and chemical stability characteristics, titanium oxide (TiO2) thin films are used in a wide range of optical applications such as electrochromic devices [98, 99].

x. Gas sensing devices fall into two major categories according to the sensing mechanism. Gas sensing mechanism can either be associated with the surface reactions or it can progress through bulk diffusion of defects. ''Surface'' sensing devices operate at moderate temperatures of 600–700 K while the ''bulk'' sensors require high temperatures of the order of 1200–1400 K. Titanium dioxide represents a thermodynamically controlled bulk defect sensor [100].

## IV. CONCLUSION

TiO2 films with anatase phase alone showing tetragonal structure were deposited by DC reactive sputtering (DCRS) technique. The TiO2 films deposited at 200oC and annealed in air at 200 and 300oC for 1 hr have been characterized for their structural optical, electrical and morphological properties. XRD results showed the presence of (101) oriented crystallites along with other small intensity peak planes (004), (112) and (211), which confirmed the deposition of TiO2 films with tetragonal anatase phase. The electrical resistivity values are about 2.0 - 8.0 x103 Ωcm. The activation energy for the TiO2 film deposited at 200oC is about 0.72 eV, whereas it is 0.60 eV for the film annealed at 300oC. EDX and XPS analysis show the formation of TiO2 films without any impurities. TiO2 films deposited at RT, 200oC and 250oC have shown direct bandgap values of 3.43, 3.41, 3.37 eV respectively showing a grain size dependence. Further, as-deposited and 200oC, 300oC annealed films showed both direct and indirect bandgap values. The refractive index value is increasing from 1.8 to 2.1 with temperature revealing densification of the TiO2 films. SEM and AFM analysis showed uniform surface morphology with grain size in the range of 100-250 nm, increasing with temperature. Raman scattering study confirmed the formation of anatase TiO2 films. TEM showed the presence of 15-30 nm sized crystallites and PL studies confirmed the formation of pure TiO2 films with direct bandgap values of about 2.96-3.30 eV.

Nano grained TiO2 films have been deposited in detail at different substrate temperatures between 300 and 500 oC using titanium acetylacetonate (TiAcAc) as the precursor metal salt. The spray solution was prepared by dissolving 0.05, 0.1, 0.15, 0.20, and 0.25 M of TiAcAc in 100% ethanol and used to prepare TiO2 films. The substrate temperature was fixed as 450oC and the molarity of TiAcAc was fixed at 0.15 M and the properties were studied. Films deposited under these conditions showed anatase phase with tetragonal structure, having the prepared orientation along (101) direction. Microstrain and grain size variations show a temperature dependent nature. The resistivity is about 104 Ωcm. The carrier concentration in about 1020–1021 cm-3 and the mobility values are very low of the order of 10-16 cm2/Vs, which is due to the high resistivity of the TiO2 films. Optical studies show that the band gap values are temperature as well as precursor concentration dependent. The direct bandgap values increased form 2.84 eV to 3.66 eV when the temperature varied from 300oC to 500oC. The refractive index value varies between about 1.9 and 2.5 in the wavelength region of 400-1000 nm. SEM and AFM morphological studies show uniform surfaces. Raman scattering and TEM studies have shown agglomerated grains with nano particles. PL studies showed a direct band gap of 3.26 eV and an indirect band gap of 2.95 eV.

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