Composite Nanostructure: An application in Dye Synthesize Solar Cell

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Abstract: The materials selected for composite preparation are ZnO and TiO$_2$, ZnO is used because it has wide range of properties that depend on doping, process parameters, fabrication methods and thickness of thin films. The properties of Zinc oxide include high transparency, piezoelectricity, wide band gap semi conductivity and sensing properties. TiO$_2$ exhibits optical, morphological, and photocatalytic behavior. The optical parameter of the ZnO was studied photoluminescence by Fluorescence spectrophotometer and structural characterization of composite was carried out by powder X-ray diffraction method. The different structure of ZnO and ZnO/TiO$_2$ were obtained by using thermal evaporation system. The Thermal Evaporator was used to achieve high vacuum. The deposition of ZnO thin film was done by taking ZnO powder high purity (99.99%) in Mo boat and was deposited on properly cleaned glass substrate by directly evaporating powder in the chamber. Similarly ZnO/TiO$_2$ composite thin film was prepared. The deposited thin film was annealed at 600°C.

Key Words: ZnO Nanostructures, TiO$_2$ Nanostructure, Composites, Dye sensitized Solar Cell

I. INTRODUCTION

The nanoscience deals with a few hundred to a few thousand atoms or atomic clusters. Nanoparticles are larger than individual atom and molecules but are smaller than bulk solid hence they obey neither absolute quantum chemistry nor laws of classical physics and have properties that differ markedly from those expected. Nanocomposite films are thin films formed by mixing two or more dissimilar materials having nano-dimensional phase in order to control and develop new and improved structures and properties. The properties of nanocomposite films depend not only upon the individual components used but also on the morphology and the interfacial characteristics. Nanocomposite films that combine materials with synergetic or complementary behaviours possess unique physical, chemical, optical, mechanical, magnetic and electrical properties unavailable from that of the component materials and have attracted much attention for a wide range of device applications such as gas sensors.

II. ZnO THE NOVEL MATERIAL

Various techniques have been used for deposition of ZnO thin film namely Pulsed Laser Deposition, Atomic Layer Deposition, DC Magnetron Sputtering, Photo Induced MOCVD, Reactive Molecular Beam Epitaxy, Molecular Beam Epitaxy etc[1]. There are merits and demerits for each deposition technique for example sputtering technique allows the fabrication of high quality films but the equipment cost is very high with a low production rate. At the same time spray techniques are very cheap but the films produced are not consistent. There is a lot of variation in the results reported by different workers using different techniques. The variation is due to the difference in the deposition parameters and the purity of the elements.

III. CURRENT SCENARIO OF TiO$_2$

As the most promising photo catalyst TiO$_2$ materials are expected to play an important role in helping to solve many serious environmental and pollution challenges. TiO$_2$ also bears tremendous hope in helping ease the energy crisis through effective utilization of solar energy based on photovoltaic and water-splitting devices. As the size, shape, and crystal structure of TiO$_2$ nanomaterials vary, not only does surface stability changes but also the transitions between different phases of TiO$_2$ under pressure or heat becomes size dependent. Titanium dioxide is available in three crystal forms:

(i) Rutile (ii) Anatase (iii) Brookite

Anatase and rutile have the same symmetry, tetragonal despite having different structures. In Rutile, the structure is based on octahedrons of titanium oxide which share two edges of the octahedron with other octahedrons and form chains[2]. In anatase the octahedrons share four edges hence the four fold axis. Crystals of anatase are very distinctive and are not easily confused with any other mineral. They form the eight faced tetragonal points.

The main use of titanium dioxide (TiO$_2$) is as a white powder pigment because of its brightness and very high refractive index. It provides good opacity to products such as paints, coatings, plastics, paper, inks, food and cosmetics. Titanium dioxide also has good ultraviolet (UV) light resistance property which helps in preventing the discolouration of plastics.
in sunlight. Sunscreens also use TiO$_2$ as a blocker because of its high refractive index and the ability to protect the skin from UV light.

IV. DEPOSITION OF THIN FILM

4.1 Deposition of TiO$_2$ layers and ZnO Thin films by electron beam evaporation

The TiO$_2$ layers and ZnO thin films were prepared in Vacuum Box coater (BC-300) by electron beam evaporation. In this high purity (99.99%) ZnO and TiO$_2$ particles were used as source materials. The substrate material is glass. We have used Mo boat for resistive heating of the sample. For boat selection, we have taken care of different parameters like reactivity, melting point, boiling point of both the boat and evaporant. The substrates were first rinsed in acetone and ethanol respectively and finally rinsed in deionized water. The substrate temperature were 200°C and 250°C respectively for deposition of TiO$_2$ layer and ZnO thin films. The deposition chamber was pumped down to 2.66*10$^{-3}$ Pa before deposition.

Deposition Methodology

![Flow chart (ZnO Thin Film Sample A)](image1)

![Flow chart(ZnO/TiO$_2$) Composite Film Sample B)](image2)

V. EXPERIMENTAL DETAILS

When a TiO$_2$ layer was deposited, the electron gun voltage and working current were 7.11 kV and 246 mA respectively. Afterwards, ZnO thin films were deposited on a glass substrate (sample A) and for the other sample (sample B) the TiO$_2$ buffer layer was deposited on ZnO thin film. The thicknesses of the TiO$_2$ layer and the ZnO thin film were 200 and 300 nm, respectively. Both sample A and B were annealed at 600°C in air for 1 hr.
5.1 Characterization of microstructure and photoluminescence of thin films

The crystal phase and crystalline orientation of the films were analyzed by an X-ray diffractometer[3]. The photoluminescence spectra were measured by Fluorescence Spectrophotometer. The excitation source was a Xe lamp for which the excitation wavelength was 325 nm. All the measurements were carried out at room temperature in air.

VI. RESULTS AND DISCUSSION

6.1 Crystalline development of the thin films using X-ray diffraction analyzer

ZnO normally forms the hexagonal (Wurtzite) structure with lattice constant (a=b=0.32 nm and c= 0.52 nm). Each Zn atom is tetrahedrally co-ordinated to four O atoms. The structural characterization of the sample was carried out by powder X-ray diffraction method performed on X-ray diffractometer Fig.3 shows the XRD patterns of ZnO and ZnO/TiO₂ thin films. The entire ZnO thin films show only one diffraction peak which corresponds to the diffraction of (002) plane of ZnO with a hexagonal wurtzite structure. The diffraction peak can also be well indexed to the hexagonal phase ZnO reported in JCPDS card (No. 36-1451, a = 0.3249 nm, c = 0.5206 nm). The results indicate that the products consisted of a pure phase. This means all the ZnO thin films deposited on the glass or TiO₂ layered substrates are preferentially oriented along the c-axis perpendicular to the substrate surface. For the sample A and B their (002) peaks lie at 34.340. From the above data, it is clear that the (002) peak positions of ZnO/TiO₂ thin films are closer to the (101) peak position of ZnO powder. According to the order of sample A and B, the intensity of their (002) peaks gradually decreases[4][5]. It means the crystalline quality of ZnO thin films is improved after TiO₂ layers are used. The average crystallite sizes of the ZnO thin films can be calculated with Scherrer formula using parameters derived from XRD patterns. Scherrer formula is as follows:

\[ D = \frac{0.9\lambda}{\beta \cos \theta} \]

Where D is the crystallite size, λ is the X-ray wavelength, β is the FWHM and θ is the diffraction angle. As regards the sample B, there is not only the (002) peaks of ZnO thin films but also two peaks of TiO₂ layers in the patterns. One of them corresponds to the (200) diffraction peak (48.30º) of anatase phase, another corresponds to the (211) peak (56.05º) of rutile phase. But the main components of TiO₂ layer are anatase structured crystals.

6.2 The Photoluminescence Property of the ZnO Thin Films

Photoluminescence is a non-destructive and contactless spectroscopic method of probing electronic structure of materials. Light is shined in the samples, which is absorbed by the sample and upon de-excitation, light is emitted by the sample which is known as photo- excitation and this mechanism is generally known as photoluminescence, i.e, light is incident upon the sample and the emitted light is collected. In order to probe the band-gap of a material, light of shorter wavelength (greater energy) is desired to excite the material. Photo- excitation causes electrons within the material, usually from valance band to move into permissible excited states[6]. When these electrons return to their equilibrium states, the excess energy is released and may include the emission of light (a radiative process) or may not (a non-radiative process). In semiconductors the most common radiative transition is between energy states in the conduction band and valance bands.

Fig.4 shows the PL spectra of the samples. From this figure, it is clear that A ZnO luminescence spectra typically consists of a sharp band at 380 nm, due to near band edge excitonic recombination and a broad green emission band in the visible range at 510 nm due to deep states inside the band gap. The stronger luminescence of the 380 nm-band relative to that of the visible emission is often considered indicative of defect-free, crystalline ZnO structures.
VII. APPLICATION IN DYE-SENSITIZED SOLAR CELL

A surface modification method was carried out by beam evaporation technique to fabricate TiO$_2$-coated ZnO electrodes (ZnO/TiO$_2$). The prepared material at nano scale level can be used as a photo-anode in photovoltaic technology for improving the performance of dye-sensitizes solar cells. The use of TiO$_2$ in dye-sensitized solar cells for the conversion of sunlight into electricity has attracted much attention because of low cost, environment friendly production and good PV efficiencies of the TiO$_2$ based solar cells. The DSSC’s usually consist of anode formed by anatase TiO$_2$ which act as an electron acceptor an absorbing layer of dye molecules which serves for harvesting of photons and injection of electrons into the TiO$_2$ anode and a liquid electrolyte consisting of some organic solvent and a redox couple I$^-$/I$_3^-$ which serves as a redox agent to reduce the photo excited dye molecules. Crystalline TiO$_2$ anode is one of the key element in this assembly. Among many possible approaches, the use of anatase one-dimensional structures is one of the promising ways, because the use of single-crystalline and one dimensional structures usually decreases interconnections between crystalline titania particles[8] . Bulk ZnO material has an energy gap close to that of TiO$_2$, it belongs to transparent conducting oxides and thus can be used either as a front or back side components in solar cells depending on the substrate. The cells are grown onto and the geometry of contacts.

VIII. FUTURE ASPECTS

Dye sensitized solar cells possess even more opportunity and space to meet upscale production and requirement of energy of practiced operation process. The overall energy conversion for a DSSC relies on the individual properties of the constituents of the cell. The choice of the semiconductor material, oxide film, nanostructures, size of pores, extent of the contact with TCO are all important factors. Thus it is necessary that these should be successfully evaluated together under an extensive experimental plan.

REFERENCES


