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An Appraisal of Optical and Structural Properties of Sm and Gd (+3 oxidation state) Doped TiO_2 and Identifying their Enhanced Efficiency by Fabricating DSSCS

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Abstract

The rare-earth elements, Gadolinium and Samarium, are doped with TiO_2 by hydro thermal synthesis technique. The obtained materials underwent the characterizations of XRD, HRTEM, UV-Vis Spectroscopy and XPS. DSSCs were fabricated using N719 dye, redox electrolyte and Platinum as counter electrode. The efficiencies of DSSCs depend on the electron transport within the TiO_2-dye-electrolyte system. After the fabrication and simulation, among the two, Gd^{3+} doped TiO_2 gives the desired outcomes and higher efficiency than the pure and Sm^{3+} doped TiO_2. Thus, it proves to be a superior solar cell anode material.

Keywords: Solar Energy; Thin Films; Samarium; Gadolinium; Dye Sensitized Solar Cells.

1. Introduction

Dye Sensitized Solar Cells are being investigated intensively as potential alternatives for the next generation solar cells. Gratzel et al reported the first DSSCs in the year 1991 and threw some light upon the increasing efficiency of solar cells with minimized expenses. DSSCs are superior to their older generation silicon solar cells in the aspects like production cost, high power conversion efficiency (PCE) and ecofriendly production [1-2].

Among all the semiconductor materials, TiO_2 nanoparticles are widely used as photoanode due to its large surface area to volume ratio, high power conversion efficiency and easy preparation in DSSCs [3]. Moreover, the conversion efficiency of TiO_2 based DSSCs have energy losses by recombination and slow electron transportation as major predicaments [4, 5]. One of the most important parts of DSSCs is photoanode [6]. However, the development of promising photo anode that exhibits better solar cell performance is still critical for the applications of DSSCs. Research works have been attempted on designing and preparing the high efficiency of materials for DSSCs. Enhancing the DSSCs' performance using TiO_2 coupling with other materials is considered to be an important field of research [7]. Such an attempt is made by doping the Rare Earth Elements like samarium and Gadolinium with TiO_2 and the characterizations were done to find the suitability of the synthesized material.

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Rare Earth Elements (REE) doped TiO_2 is synthesized through hydrothermal method and produced as an efficient photo anode. The effect of Samarium (Sm^{3+}) and Gadolinium (Gd^{3+}) on the surface and morphology of TiO_2 was investigated by characterizing the material with XPS, TEM and XRD. The optical property was elucidated by UV spectroscopy. The J-V characteristic provides the data to calculate the efficiency of the fabricated DSSCs. Doping TiO_2 with transition metals is known to enhance their response in visible light region [8]. Very few reports are available accounting for the improvement in the efficiency of TiO_2 towards visible light when doped with lanthanide ions/oxides [9]. Study on the comparison of doping Sm^{3+} and Gd^{3+} (2wt %) with TiO_2 is not commonly available in works hence this work will pave path for the researchers to explore more.

2. Experimental selections

Samarium (III) Oxide (powder, Sm_2O_3, 99.9%), Gadolinium (III) Oxide (powder, Gd_2O_3, 99.9%) and Ethanol (99%) were purchased from Merck. Titanium (IV) Isopropoxide (liquid, $Ti[OCH(CH_3)_2]_4$, Anatase, 99.9%), Platinum (liquid, 99.9%), Fluorine doped tin oxide (FTO, 13 Ω/sq) coated glass were received from Sigma-Aldrich. All chemicals were used as such without further purification.

3. Preparation Technique:

Solution reaction-based approach is carried out to synthesize Nano materials and this method has good control over the compositions of the synthesized nanomaterials. Solution of Pure TiO_2 and Rare Earth Element (Sm^{3+}/Gd^{3+}) doped TiO_2 were synthesized using this widely employed technique. Titanium (IV) isopropoxide (anatase, 99.9%) and acetic acid were taken in 1:4 molar ratio. Drop by drop, 20M of distilled water was added to the solution during magnetic stirring to get the solution. This process is allowed for 25mins to observe better results. The obtained solution was poured into a Teflon autoclave. The autoclave was placed in the furnace at 100^{o}C for 24 h. The product was exposed for 3h at the heating rate of 5°C/min to obtain TiO_2 nanoparticles by calcination at 400°C. Similarly RE^{3+} doped TiO_2 samples were synthesized by introducing Samarium (2wt %) to the solution during the stirring process. Similarly Gadolinium (2wt%) was doped with TiO_2 adhering to the above process. All chemical reagents are used without further purification as they were obtained from commercial sources with the highest purity.

4. Results and Discussions:

4.1 XRD

The prepared samples' crystallographic phases were investigated using XRD. Figure 1(a,b,c) explicates the presence of strong diffraction peaks at $2\theta \approx$ 25.2°,37.9°,48.1°, 54.1°,54.9°,62.7°,68.9°,70.1° and75.1° have (101), (004), (200), (105), (211), (204), (116), (220) and (215) as corresponding reflections. The ratio of the different peaks indicate that the arrangement is uniform and symmetrical. Anatase crystalline structure is present and the studies authenticate that there is no other crystalline structure of titania observed. Size of the material is reduced in the doped particles was determined using the prominent peak observed at 25.2°. The size of the grains were 9.2nm for pure, 7.77nm for Sm^{3+} and 7.74nm for Gd^{3+} doped TiO_2 calculated from the plane 101 utilizing Scherrer's equation.

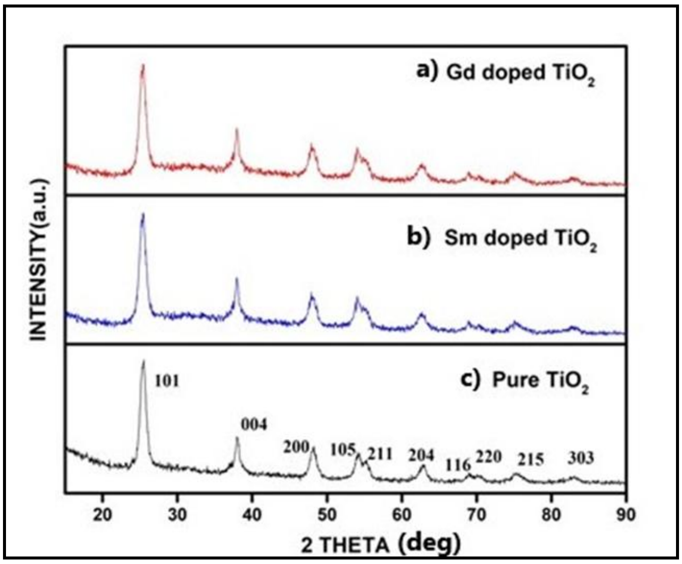

Fig. 1. Figure 1: XRD images of a) Gd Doped b) Sm Doped c) Pure TiO_2

4.2 HR-TEM

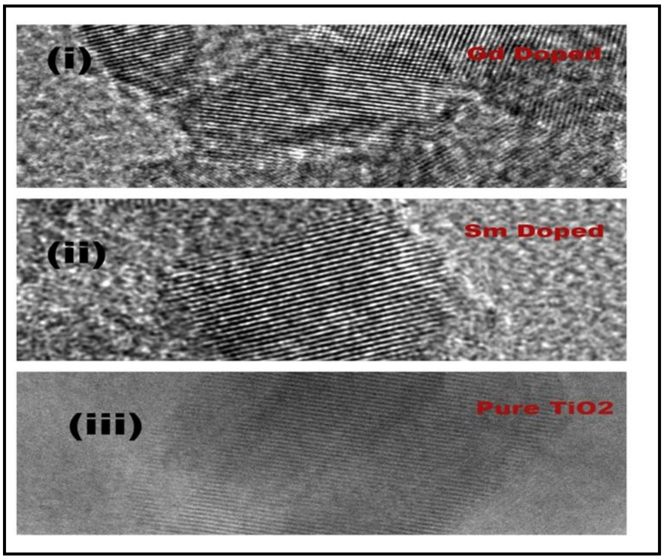

Figure 2: High Resolution TEM images of i) Gd Doped ii) Sm Doped iii) Pure TiO_2

Figure 2 depicts the HRTEM images of Gd Doped, Sm Doped, andPure TiO_2 nanoparticles.

4.3 Absorption Spectra

Figure 3 a) denotes the optical absorption spectra of TiO_2 and Sm^{3+} and Gd^{3+} doped TiO_2 respectively. 2.94eV, 2.85eV and 2.83eV are the optical bandgap values of pure TiO_2, Sm^{3+} doped TiO_2 and Gd^{3+} doped TiO_2 respectively. The Fermi level reduction is a significant cause for bandgap reduction. As the Fermi level reduces the conduction of the material increases. The results show that Gd doped TiO_2 is more active in UV-A, UV-B and visible spectrum region than Sm doped or Pure TiO_2 and absorb light to enhance the photovoltaic conversion.

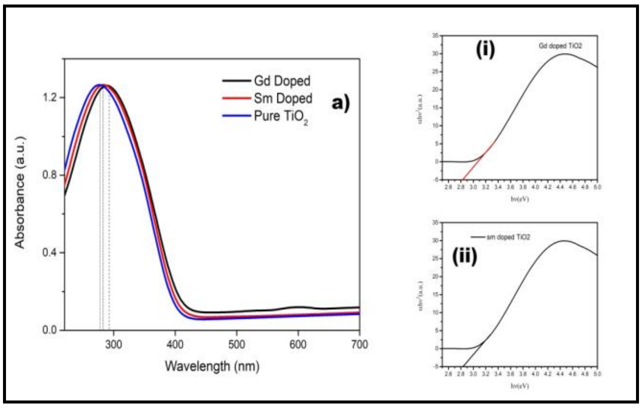

Figure 3 a) Absorption Spectra of (i) Gd Doped and (ii)Sm Doped TiO_2

4.4 XPS

High Resolution XPS study of the synthesized samples are given in Figure4(a-c). The wide graphs of doped materials in Figure 4a) assures the presence of Ti, C, O, Sm^{3+} and Gd^{3+}, moreover, the impurities are not much evident here. It also illustrates the presence of $Sm3d_{5/2}$ and $Gd3d_{5/2}$ on the surface. Figure 4b) assures the presence and location of $Ti2p_{3/2}$ and $Ti2p_{1/2}$ at 458.56eV and 464.22 eV for Sm^{3+} and Gd^{3+} doped TiO_2 samples. The findings are in conformity with the reference data results that the tetravalent Ti atoms are consistent in TiO_2 lattice. This also proves that Gd^{3+} doped material has higher binding energy than Sm^{3+} doped.

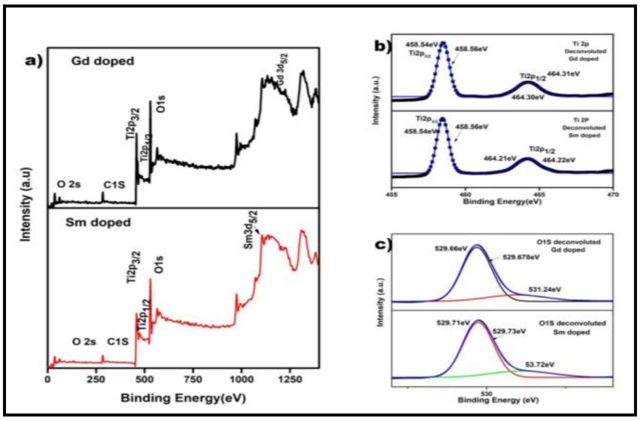

Figure4: XPS Spectra of Sm and Gd Doped TiO_2

O1s configuration peaks, observed in Figure3c) are the results of oxygen presence on the surface in crystal lattice. The peaks are observed at 529.66eV for Gd and 529.71eV in Sm. The impurity energy level between O2p orbital and Ti3d orbital is increased by the presence of Sm^{3+} and Gd^{3+} ion in the TiO_2 nano particles, which in turn narrowed the charge transfer band. Hence XPS analysis is in conformity with XRD and HRTEM studies regarding surface morphology.

4. 5 Preparation of DSSC:

Employing FTO glasses as substrates, 0.1g of prepared materials (TiO_2, Sm^{3+}/Gd^{3+}) added with Triton X100 and ethanol were coated by spin coating technique. Then it is left to dry at the ambient temperature. On the anode FTO glass, 5mmol of N719 dye was applied and left to spread evenly for 12hrs. A few drops of liquid platinum were placed on another FTO glass and left to spread evenly. It was exposed to 350°C for 25mins to obtain the Platinum counter electrode. The two electrodes were sandwiched and through a hole made on the counter electrode. I^-/I_3^- taken as electrolyte were injected. The arranged system was placed in the simulator to measure the activity of DSSC. At room temperature using a Keithley 2400 high current source power meter under white-light illumination from a 500 W Xenon lamp (AM1.5G) Current density–Voltage (J–V) measurements were taken.

5. I-V Characteristics

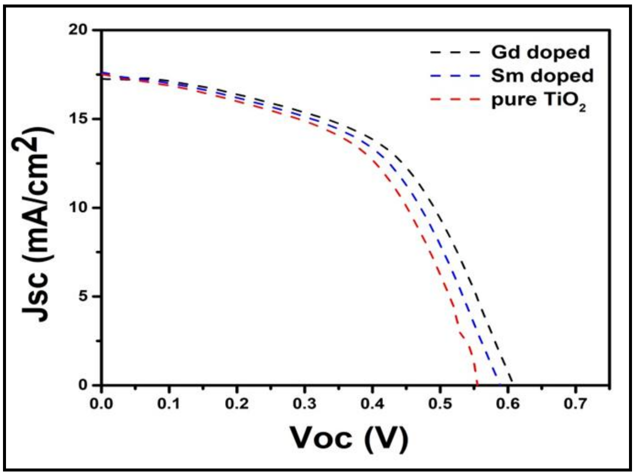

Figure 5: IV Curve

Current Density-Voltage performances of Pure, Sm^{3+} and Gd^{3+} doped TiO_2 DSSCs are provided in Table1 and the curves are portrayed in Figure 5. The conversion efficiency was high for Gd^{3+} doped TiO_2 compared to Sm^{3+} doped and pure TiO_2. One of the salient factors for the enhancement of the efficiency is the increase in UV and Visible region light absorption of the materials. As the band gap decreases the conduction of Gd^{3+} doped TiO_2 increases.

Table 1: Efficiency of DSSCs (PureTiO_2, Sm doped and Gd Doped TiO_2)

Sample	J_{sc} (mA/cm²)	V_{oc} (V)	J_{max} mA	V_{max} (V)	(FF)	η (%)
TiO_2	17.24	0.56	0.3650	13.71	0.5183	5.003
Sm^{3+} + TiO_2	17.25	0.58	0.3830	13.75	0.5263	5.265
Gd^{3+} + TiO_2	17.25	0.605	0.3971	13.96	0.5311	5.542

6. Conclusion

Sm^{3+} and Gd^{3+} doped TiO_2 were synthesized with spin coating technique. Morphological and optical properties of the materials were characterized. After the elaborate analysis, the prepared anode materials were converted into electrodes and respective DSSCs were constructed. Among the samples, Gd^{3+} doped TiO_2 exhibited reduced size, 7.74nm, minimized bandgap, 2.91eV and greater absorption of solar light and better efficiency of 5.542%. These results vouch that Gd^{3+} doped TiO_2 is an apt anode material than Sm^{3+} doped TiO_2 for the assembling of DSSCs.

Conflict of Interest: Nil

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