International Journal of Scientific Research and Engineering Development-– Volume 5 Issue 2, Mar-Apr 2022

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RESEARCH ARTICLE OPEN ACCESS

Doping of Cr in TiO_2 Creates Variation in Energy Band Gap Value for Enhancing its Application in Photovoltaic

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Abstract:

TiO_2 nanopowders doped with Chromium (Cr) are prepared by Titanium isopropoxide (TTIP) and methanol using simple sol-gel method. Cr powder of different concentration is doped during the preparation of TiO_2. The prepared specimens of TiO_2/(0.2g)Cr and TiO_2/(1.0 g)Cr is annealed at 500^0C and 700^0C for 1 hour in air. TiO_2 exhibits pure anatase phase along with Cr peaks for the specimen annealed at 500^0C whereas the specimen annealed at 700^0C contains TiO_2 in mixed anatase and rutile phase with Cr peaks as revealed by X-ray diffraction pattern (XRD). The average crystallite size of TiO_2/Cr nanopowder increases with increase in annealing temperature and energy band gap values are obtained by extrapolating linear region of Tauc plot to X-axis. The doping of Cr reduces energy band gap value as 2.28 eV for TiO_2/(0.2g)Cr-500^0C and 1.89 eV for TiO_2/(0.2g)Cr-700^0C. This change in band gap value shifts optical absorption of TiO_2 in the visible spectral region in the solar spectrum which may play an important role for photon absorption. Therefore photo anodes may be fabricated using TiO_2/Cr nanopowder which enhances its application in photovoltaic.

Keywords — Band Gap, Chromium, Titanium, Doping, Photovoltaic

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I. INTRODUCTION

Titanium dioxide (TiO_2) is one of the widely used materials due to its excellent optical properties and high chemical stability [1, 2]. It mainly exists in three phase anatase, rutile and brookite. Anatase and brookite are metastable phases while rutile is the most stable phase. The energy band gap values of anatase and rutile phases are 3.2 eV and 3.0 eV respectively [3, 4]. TiO_2 is extensively used for solar energy applications because of its optoelectronic and photochemical properties. However, the large band gap of TiO_2 hinders the utilization of solar spectrum [5-7].

In order to improve photovoltaic properties of TiO_2, it is highly desirable to work on the reduction of energy band gap value. Doping of an element in TiO_2 is one of the simple techniques to achieve different results such as creation of charge carriers, formation of new valence states in TiO_2 and band gap value reduction [7]. The main focus of the present study is to develop a TiO_2 based material with reduced energy bang gap. Therefore in this investigation Chromium (Cr) doped titanium dioxide (TiO_2) nanopowder is prepared by simple sol-gel method which may be used to develop photo anodes for photovoltaic applications.

II. MATERIALS AND METHODS

TiO_2 doped with Cr nanopowders are prepared by sol-gel method. In our investigation the preparation method of TiO_2 is optimized by varying concentration of Titanium isopropoxide (TTIP) which is used as starting material [2]. 0.2 g and 1.0 g Cr metal powder is added into the mixture of titanium isopropoxide and methanol. The solution is heated at a temperature of about 57 ± 3^0C and stirred vigorously using magnetic stirrer. The gel is kept for 12 hours at room temperature for drying. The TiO_2/Cr powder thus obtained is annealed at 500^0C and 700^0C respectively for 1 hour in air. Hence TiO_2/ (0.2g)Cr and TiO_2/(1.0g)Cr powders produced are characterized by X-ray diffraction pattern (XRD) to study the phases and crystallite size.

III. RESULTS AND DISCUSSION

The X-ray diffraction patterns (XRD) of TiO_2/(0.2g)Cr and TiO_2/(1.0g)Cr nanopowders are shown in Fig.1 (a) and Fig. 1 (b). CuK_α radiation is used to record X-ray diffraction pattern (XRD) and diffraction angles are in good agreement with JCPDS no 21-1272 for anatase, JCPDS no 21-1276 for rutile and data reported in the literature [2, 5]. The average crystallite size for TiO_2/Cr nanopowders are calculated using Scherrer's formula [5].

$$D= 0.89\,\lambda / \beta \cos\theta \qquad (1)$$

where D is crystallite size in nanometer, β is the full width at half maximum (FWHM) in radian, λ is the wavelength of the X-ray which is 0.15406 nm for Cu target Kα radiation and θ is the Bragg angle.

Fig. 2 (a) and Fig. 2 (b) depicts Tauc plots obtained by U V absorption spectra recorded by Shimadzu UV-1800. The energy band gap values are calculated by extrapolating linear region of Tauc plot to X-axis [8]. The calculated energy band gap values, average crystallite size and percentage content of anatase/ rutile phase of TiO_2/Cr nanopowders are summarized in Table 1.

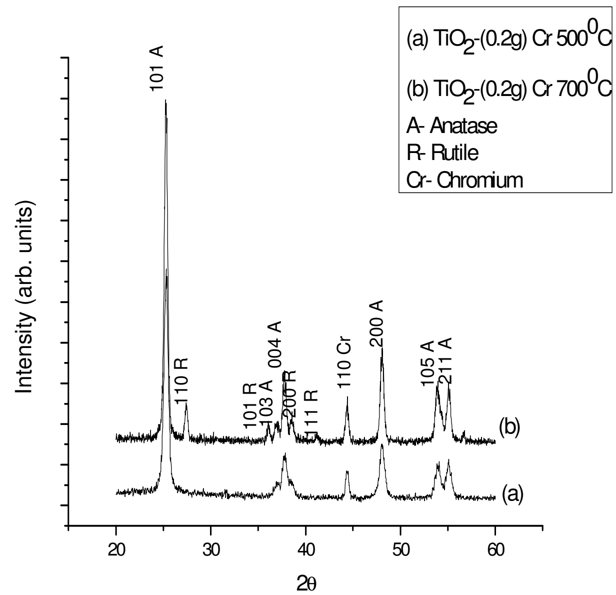

Figure 1 (a)

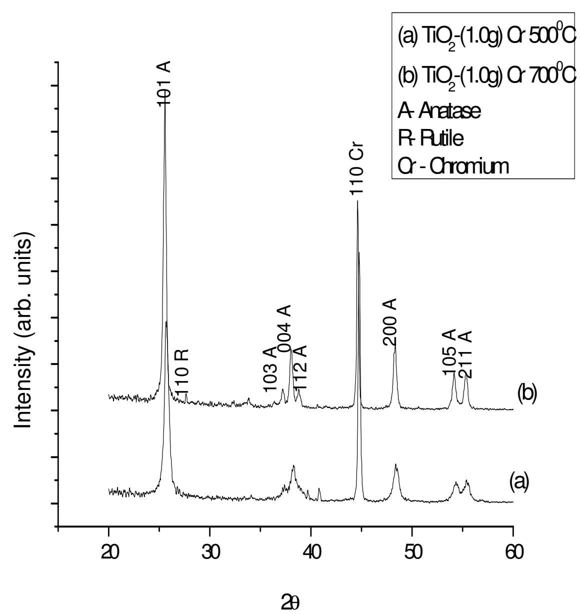

Figure 1 (b)

Figure 1. X-ray diffraction pattern of (a) TiO_2-0.2g Cr and (b) TiO_2-1.0g Cr specimens

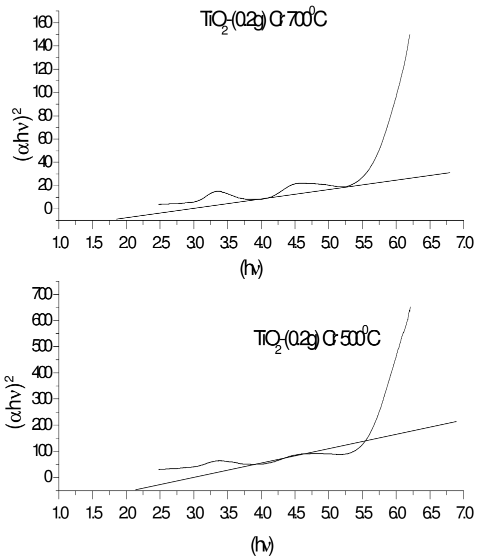

Figure 2 (a)

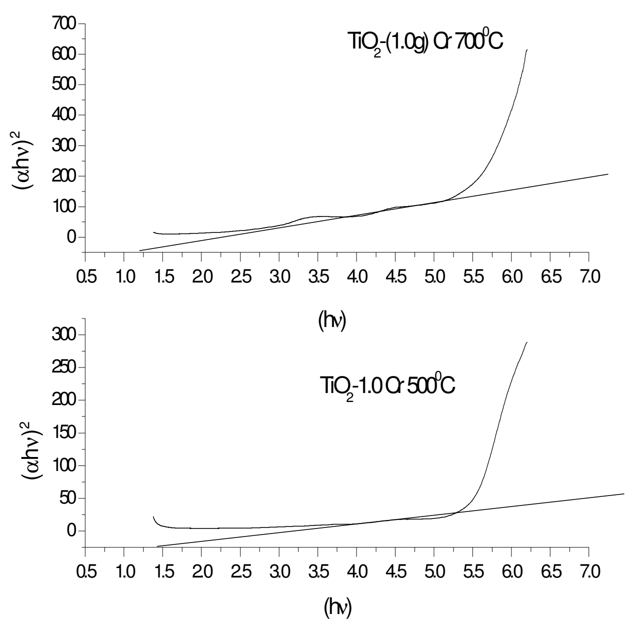

Figure 2 (b)

Figure 2. Tauc plot of (a) TiO_2-0.2g Cr and (b) TiO_2-1.0g Cr specimens

Table 1. Various parameters of TiO_2-0.2g Cr and TiO_2-1.0g Cr specimens

	TiO_2-0.2g Cr 500^0C	TiO_2-0.2g Cr 700^0C	TiO_2-1.0g Cr 500^0C	TiO_2-1.0g Cr 700^0C
Average Crystallite Size	15±5 nm	30±5 nm	15±5 nm	30±5 nm
Intensity I_a (101 anatase)	-	4934	-	680.03
Intensity I_r (110 rutile)	-	1258	-	36.67
% Anatase	-	76%	-	94%
% Rutile	-	24%	-	6%
Energy Band Gap Value	2.28 eV	1.89 eV	1.5 eV	1.27 eV

The X-ray diffraction pattern (XRD) of TiO_2/(0.2g)Cr and TiO_2/(1.0g)Cr nanopowders annealed at 500^0C shows pure anatase phase while specimens annealed at 700^0C of TiO_2/(0.2g)Cr and TiO_2/(1.0g)Cr nanopowders depicts both anatase and rutile phase. The presence of Cr peaks confirms the doping of Cr in TiO_2 nanopowder. The average crystallite size of TiO_2/Cr nanopowders increases with increase in annealing temperature as seen from Table 1. It is also observed that percentage content of rutile phase decreases with increase in doping concentration of Cr. The energy band gap value of TiO_2/Cr nanopowders are significantly reduced as compared to pure TiO_2 due to Cr doping. Therefore this may lead to shift in optical absorption of TiO_2 in the visible spectral region of solar spectrum.

Loan et al. reported that doping of Cr^{3+} into the TiO_2 lattice creates Schottky barrier which improves the transfer of electrons from TiO_2. This may lead to significant changes on the electronic structure of a crystalline material and may affect energy band gap values [9]. In another investigation Li et al. proposed that doped Cr^{3+} ions can replace Ti atoms in the lattice to compensate oxygen vacancy and distribute homogeneously within TiO_2 crystals which results in the absorption of visible light [10]. In the light of data reported in the literature the TiO_2/Cr nanopowders exhibiting reduced energy band gap values may play an important role for photon absorption. Therefore TiO_2/Cr nanopowders may behave as a suitable candidate to develop photo anodes which enhances its application in photovoltaic.

(IV) CONCLUSIONS

1. The doping of Cr in TiO_2 reduces its energy band gap value which shifts optical absorption of TiO_2 in visible region.

2. TiO_2/Cr nanopowders may be used to fabricate photo anodes for photovoltaic applications.

ACKNOWLEDGMENT

Authors thank Science & Engineering Research Board (SERB) for providing financial grant vide no SERB/F/5303/2014-15 and Nanoscale Research Facility (NRF) Centre, IIT Delhi for XRD facility.

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