

# Growth and Characterization of TiO<sub>2</sub>-CaO Nanocomposite Thin Film Solar Cells

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## Abstract

Titanium dioxide (TiO<sub>2</sub>) – calcium oxide (CaO) nanocomposite was prepared by solid state reaction route. The composite was characterized by x-ray diffraction (XRD) and scanning electron microscopy (SEM). The mixed powder was deposited onto silicon (Si) substrate by spin coating technique. The Photovoltaic behavior of thin film solar cell under illumination was examined by I-V (current-voltage) characteristics curve.

**Key words:** Photovoltaic, nanocomposite, XRD, SEM, solar cell

## Introduction

Photovoltaic (PV) cells are devices that convert sunlight to electricity by passing thermodynamic cycle and mechanical generators [Minami T, et al, 2000]. Thin film photovoltaic aim to reduce the cost per unit energy of electricity generated from sunlight compared to conventional silicon solar cells [Lin L.Y, et al, 2011]. Several approaches have been developed for solar cells such as amorphous and nanocrystalline Si, inorganic compound semiconductors, quantum dot solar cells (QDSCs), dye-sensitized solar cells (DSSCs), organic solar cells (OSCs) and perovskite-base meso-superstructure solar cells (MSSCs) [Wang J.T, et al, 2013]. In this research work, the porous semiconductor film TiO<sub>2</sub>-CaO layer consists of a large collection of nano-size particles of a metal oxide introduced by nano-sized pores, deposited onto the conductive surface of a silicon. This porous metal oxide film acts as a high surface area support for a path way for electrical current and porous membrane for diffusion of the redox couple [Park K.H, et al, 2008]. The high surface area of the nanocrystalline TiO<sub>2</sub>-CaO film plays a crucial role in increasing the performance of the photoelectrochemical cell in the energy conversion. Therefore, mesoporous TiO<sub>2</sub>-CaO are expected to facilitate pore diffusion, give easier access to the film surface, and allowed the nanocrystal junction to be formed wider batter control.

## 2.Experimental

### 2.1 Powder Preparation

To prepare the TiO<sub>2</sub>-CaO nanocomposite, titanium dioxide and calcium oxide were used as starting materials. First of all, pure TiO<sub>2</sub>, the mixture of TiO<sub>2</sub> (95%) – CaO (5%) and the mixture of TiO<sub>2</sub> (90%) – CaO (10%) powders were weighed according to their respected compositions. Each of these samples was placed in clean agate mortar and ground with a pestle for 3 h each to form homogeneous. Later, sieved it with a 3-stage mesh sieves to become uniform grain size and ball-milled for 3h to reduce the particle size. And then the samples were separately annealed at 800°C for 1h. All samples were examined by X-ray diffraction (XRD) and scanning electron microscopy (SEM) in order to analyze the structural and microstructural properties.

### 2.2 Solvental Solution

A few ml of 2-methoxyethonal solvent was added into the respective powders. They were placed in beaker and stirred by heating magnetic stirrer at 840 rpm for 2 h each.

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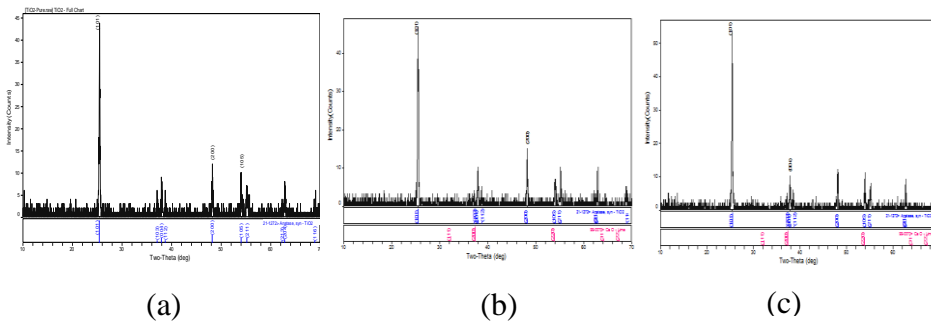
## 2.3 Film Deposition

Before spin coating, 1cm×1 cm silicon (Si) substrates were cleaned by large scale silicon cleaning process and dried at room temperature. In spin coating process, the constant spin rate of 1000 rpm and 30 s spinning time were set for the process. Finally, the fabricated layers were heated at 500°C for 1 h. After that, the films fabricated were analyzed by XRD to examine the film characterizations.

## 3. Results and Discussion

### 3.1 XRD Analysis of powder

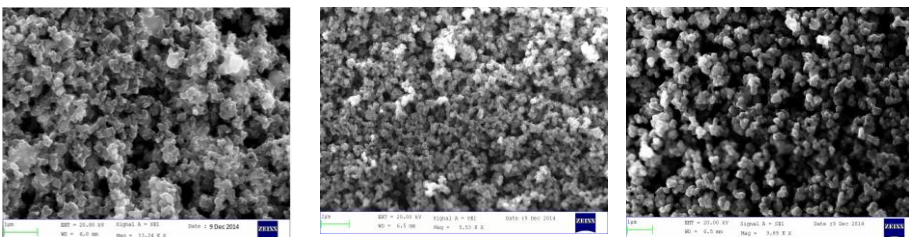
The XRD patterns of pure TiO<sub>2</sub> (TO), TiO<sub>2</sub> (95%)- CaO (5%) (TCO5) and TiO<sub>2</sub> (90%)-CaO(10%) (TCO10) powders were shown in Fig 1(a, b & c). The diffraction peaks were identified by using the standard powder diffraction data of TiO<sub>2</sub>. The samples were scanned from 10° to 70° in 2θ with a step size of 0.01. Among all the profiles, (101) was the most prominent peak and the others were matched on the standard profile of pure TiO<sub>2</sub>. The lattice parameters and crystallite sizes were evaluated in Table 1. From the results, the phase assignment of TCO composite was the same as that of TO (tetragonal). The lattice distortion (c/a) were 2.4837, 2.5045 and 2.5200 for TO, TCO5 and TCO10. And then, the lattice matches were 97.3%, 93.8% and 99.07% respectively. So the undoped TO and composite TCO exhibits good crystallographic properties and crystalline behavior.



**Fig. 1** XRD spectrums of (a) TO (pure) powder , (b) TCO5 powder and (c) TCO10 powder

### 3.2 SEM Analysis of powder

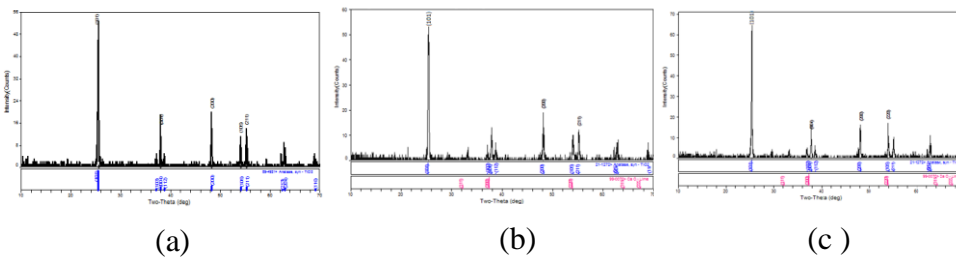
The microstructural properties of powder samples were analyzed by scanning electron microscopy (SEM) and illustrated in Fig 2 (a, b & c). All SEM images were fairly dense and slightly difference with one another. Grains were uniformly distributed and circular in shape. The morphological change was observed by adding the CaO. The average grain sizes were 0.3621 μm, 0.1514 μm and 0.1843 μm for TO, TCO5 and TCO10. The data result from SEM images , all the samples were quite suitable for growth chemistry.



**Fig. 2** SEM images of (a) TO powder , (b) TCO5 powder and (c) TCO10 powder

### 3.3 XRD Analysis of Thin Film

To observe the phase identification and crystallographic properties of TiO<sub>2</sub>-CaO film the XRD analysis was used. The XRD profiles of undoped TO, TCO5 and TCO10 films were shown in Fig 3(a-c). From Fig 3 (a), five diffracted peaks were clearly formed on observed profile and matched with the standard (or) reference TiO<sub>2</sub> (89-4921> Anatase, syn- TiO<sub>2</sub> library file). Some extra peaks were appeared on observed spectrum and they could not be identified. From Fig 3(b), three diffracted peaks (101), (200) and (211) peaks were matched with those of TiO<sub>2</sub> standard (21-1272> Anatase, syn- TiO<sub>2</sub>). From Fig 3 (c), four diffracted peaks were appeared on observed XRD. Three identified peaks such as (101), (004) and (200) were matched with those of TiO<sub>2</sub> standard (21-1272> Anatase, syn- TiO<sub>2</sub>) while (220) peak was matched well with that of CaO standard (99-0070> CaO-lime). Therefore, CaO (10%) is enough to make TiO<sub>2</sub> (90%) - CaO (10%) composite film at 500 °C. The crystallite sizes of TO and TCO films were described in Table 1. From the film analysis by XRD, undoped TO, TCO5 and TCO10 nanocomposite films exhibited anatase titania crystal, rutile phase could not be detected at given substrate temperature at 500 °C. This meant that the small amount of CaO didn't change the structure of anatase- TiO<sub>2</sub>.



**Fig. 3 XRD spectrums of (a) TO (pure) film , (b) TCO5 film and (c) TCO10 film**

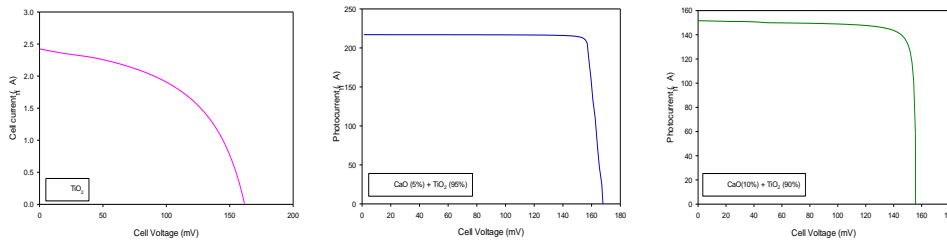
**Table. 1 Lattice parameters of sample powders and films from XRD profiles**

samples	Lattice parameters		FWHM of (101) plane (deg)	Crystallite size of (101) (nm)
	a (Å)	c (Å)		
TO powder	3.7711	9.2714	0.154	52.888
TCO5 powder	3.7728	9.4394	0.254	32.061
TCO10 powder	3.7731	9.5024	0.113	72.062
TO film	3.7459	9.4600	0.186	43.789
TCO5 film	3.7757	9.4015	0.189	43.086
TCO10 film	3.7706	9.4991	0.148	55.021

### 3.4 Illumination I-V characteristics of TiO<sub>2</sub> - CaO Thin Film Solar Cells

To examine the photovoltaic performance or solar cell evaluation of undoped TiO<sub>2</sub>, TiO<sub>2</sub>-CaO composite films, current and voltage (I-V) characteristic were measured under illumination condition. Fig 4 (a-c) showed the change in current flow as a function of cell voltage under illumination for undoped TO, TCO5 and TCO10 films. All graph natures indicated the solar cell or photovoltaic behavior. By projection from tangential point onto Y-axis (current axis) of illuminated I-V

curve, the current at maximum power point ( $I_m$ ) was obtained while the projection onto X-axis (cell-voltage axis) the voltage at maximum power point ( $V_m$ ) was formed. The open circuit voltage ( $V_{oc}$ ), short circuit current ( $I_{sc}$ ),  $I_m$  and  $V_m$  were collected and listed in Table 2. The conversion efficiencies were calculated to be 1.0029 %, 1.9956 % and 1.2378 % for undoped TO, TCO5 and TCO10 films. The fill factor values were also determined to be 0.874, 0.893 and 0.854 for respective films. Table 3 showed the conversion efficiency and fill factor for respective films.



Samples	Conversion efficiency $\eta$ (%)	Fill factor ( $F_f$ )
TO(pure) film	1.00	0.87
TCO5 film	1.99	0.89
TCO10 film	1.24	0.85

**Fig.4 (a) I-V characteristic curve for TO (pure) film , (b) I-V characteristic curve for TCO5 film and (c) I-V characteristic curve for TCO10 film**

**Table 2.  $V_{oc}$ ,  $I_{sc}$ ,  $I_m$  and  $V_m$  of all PV cells**

Samples	$V_{oc}$ (mV)	$I_{sc}$ ( $\mu A$ )	$I_m$ ( $\mu A$ )	$V_m$ (mV)
TO (pure) film	161.440	2.41	1.78	110.960
TCO5 film	168.012	217	211	154.512
TCO10 film	155.628	152	140	144.792

**Table 3. The conversion efficiency ( $\eta_{con}$ ) and fill factor ( $F_f$ ) of all PV cell**

### Conclusion

The preparation of  $TiO_2$ -CaO (TCO) solar cells have been successfully investigated. From XRD analysis, The phase assignment of TCO composite was the same as that of pure

TiO<sub>2</sub> (tetragonal). From SEM analysis, the grains were exact and crowded circular smooth and non-creasing. From the film analysis by XRD, undoped TO, TCO5 and TCO10 nanocomposite films exhibited anatase titania crystal at 800 °C. And also, the reaction temperature 800 °C and substrate temperature 500 °C chosen in this study are quite optimized temperatures. Illuminated I-V characteristic curve revealed the photovoltaic nature of fabricated films for undoped TiO<sub>2</sub> and TiO<sub>2</sub>-CaO nanocomposites. This curve also showed the V<sub>oc</sub> -I<sub>sc</sub> (open circuit voltage – short circuit current) reached its maximum value, vice versa. Actually, V<sub>oc</sub>-I<sub>sc</sub> curve came from the 4<sup>th</sup> quadrant of the circle. By rotating this curve by 180 deg through the current axis, illuminated I-V curve was formed in the 1<sup>st</sup> quadrant of the circle. The conversion efficiency was determined to be 1.0029 %, 1.9956 % and 1.2378 % for undoped TiO<sub>2</sub>, TiO<sub>2</sub>(95%) -CaO (5%) and TiO<sub>2</sub> (90%)-CaO (10%) composite films. All fill factors were ranged between 0.85 to 0.89 and satisfied the industrial realization. According to the analytical results of XRD and SEM, it is concluded that the preparative steps and experimental trends in this research work are cost effective, unsophisticated and non-complicated for composite fabrication technology. The experimental data resulted from this research work is credible and applicable in use for low-cost Si-based thin film solar cell.

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