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Studies on *n*-TiO_2/*p*-Si structure for solar cell applications

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Abstract : Titanium dioxide (TiO_2) and Silicon (Si) are two types of materials that have been widely investigated for sensors and solar cell applications. Nanocrystalline TiO_2 thin film has been successfully deposited on *p*-type silicon wafer by sol-gel spin coating method. The structural, surface morphological and optical properties were characterized by XRD, SEM and PL studies. XRD results confirm the formation of good crystalline quality TiO_2 tetragonal structure on silicon surface. Along with dominantsilicon peak, anatase& rutilepeaks of TiO_2 were also observed. Thecalculated grain size for TiO_2/Siheterostructure was 32 nm. SEM image showshomogeneous island like structures.Elemental composition of the film wasinvestigated using EDAX study. Blue and green emission peaks were observed at an excitation of 410 nm in PL spectrum. These results show that the described technique is a cost effective method for fabrication of TiO_2/Si structure.

Keywords – TiO_2/ Si structure, Spin coating method,XRD, PL, SEM and FTIR.

Introduction

Metal oxide–semiconductor(MOS)structure can be used in many areas such as switching devices,sensors, solar cells and so on[1].The MOS structure is one of the most important heterojunction usedin photovoltaic technology.Oxide insulating layers such as Al_2O_3, SnO_2, SiO_2 and TiO_2[2]are widely used in MOS structures. Among these oxide insulator materials, TiO_2 has received considerable interestdue to virtue of its excellentchemical stability, non-toxicity, low cost, large band gap (3-3.2 eV) and remarkable electrical and optical properties. Coatings ofTiO_2 thin film on Si wafer creates a continuous surface state distribution at semiconductor–oxide insulator interface. Nanocrystalline TiO_2 films prepared bysol-gel processhas many advantages like cost effective method, excellent control over chemistry, homogeneity and purity[3]. In the present work,structural, surface morphological and optical properties of TiO_2 thin film coated over Si substrates were studied in view of solar cell application.

Experimental Details

TiO_2 sol was prepared using titanium tetra isopropoxide (TTIP), ethanol (as solvent) and acetylacetone. 1 ml of TTIP was mixed with 10 ml of ethanol and stirred for 10 minute using magnetic stirrer to obtain a milky white solution. To this mixture 1 ml of acetylacetone was added and stirred for 30 minute to obtain an orange coloured solution. Again 10 ml of ethanol was added to the solution and stirred vigorously for 3 hours. The prepared sol was kept in an open air for 48 hours for aging and the gel is formed.To coat the TiO_2 film the gel was dropped onto the silicon substrate, rotated at a speed of 3000 rpm for 10s by using the spin coater. The substrate was then dried at $150^{o}C$ for 10 minute in a muffle furnace. The process of spinning and drying was repeated for seven more times to obtain aneight layer coated film. Finally the coated films were annealed at 550°C for 1 hour.

Nanocrystalline TiO_2 thin films coated on Si were subjected to XRD, Photoluminescence, SEM with EDAX and FTIR analysis. The crystallites of TiO_2 thin films coated on Si were characterized by X– Ray diffraction (XRD) using X'PERT PROX – ray diffractometer which was operated at 40 KV and 30 mA with $CuK\alpha_1$ radiation of wavelength 1.5406Å. The photoluminescence (PL) spectrum were recorded using CARY ECLIPSE instrument with Fluorescence lamp as the light source at room temperature with an excitation wavelength of 410 nm. Surface morphology and elemental analysis of the film were studied using VEGA 3 TESCAN.The Fourier Transform Infra-Red (FTIR) spectrum of the samplewas recorded using the SHIMADZU IR affinity-1 spectrophotometer in the range of 400–1500 cm^{-1}.

Results and Discussion

Structural analysis

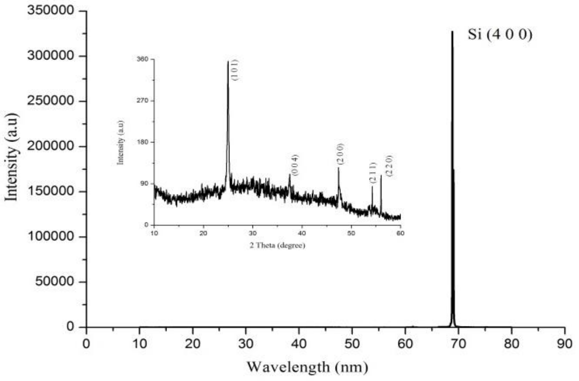

Figure 1 XRD pattern of TiO_2/Si structure

Figure 1 shows the XRD pattern of TiO_2 thin films annealed at 550°C with 8 coatings. The most dominant peak at $2\theta=68.89^\circ$ corresponds to the reflections from (4 0 0) set of planes (JCPDS File No. 89-2955) and is due to crystalline Si substrate. The other TiO_2 peaks with (1 0 1),(0 0 4), (2 0 0)and (220) orientation corresponds toanatase phase(JCPDS file No.21-1272) and (2 1 1) orientation corresponds to rutile phase(JCPDS file No.21-1276).All these peaks belong to tetragonal crystal structure. The crystallite size was determined using the well-known Debye- Scherrer's formula,

$$D = \frac{k\lambda}{\beta \cos\theta} \qquad (1)$$

where k= 0.94, λ= 1.5406Å, β= Full Width Half Maximum (FWHM) and θ= Diffracting angle.The crystallite sizecalculated forTiO_2/Si structurewas 32 nm.Based on the XRD data the percentage of anatase and rutile phases were calculated using the followingequation[4]

$$\text{Anatase (\%)} = \left[\frac{0.79 I_A}{\left(I_R + 0.79 I_A \right)} \right] \times 100 \qquad (2)$$

$$\text{Rutile (\%)} = \left\{ \frac{1}{\left[\frac{I_R + 0.79 I_A}{\left(I_R \right)} \right]} \right\} \times 100 \qquad (3)$$

where I_A and I_R are the peak intensities of (1 0 1) and (2 1 1) reflections for anatase and rutile phase respectively. The calculated percentage of anatase and rutile phase of TiO_2/Si structurewas 77% and 23%.

SEM and EDAX analysis

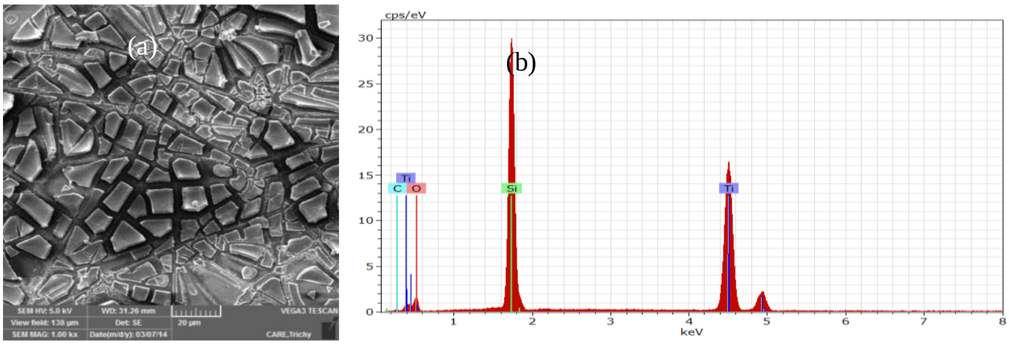

Figure 2(a)&(b) SEM image and EDAX spectrum of TiO_2/Si structure

The surface morphology and EDAX spectrum TiO_2/Si structure annealed at 550^{o}C with 8 coatings are shown in Figure2(a) &(b).SEM image shows that a thin sheet of layer is attached on the top of the Si surface with islands and small canals with non homogeneous mosaic like structures. The elemental analysis by EDAX study (Figure 2(b)) shows that the TiO_2 thin film coated on silicon substrate is mainly composed of Ti, O and Si elements.

Photoluminescence analysis

From the Figure 3 the blue and green emission peaks are observed at 490 & 530 nm. The emission peak at 490 nm is attributed to impurities and defects and the peak at 530 nm is due to oxygen vacancies[5].

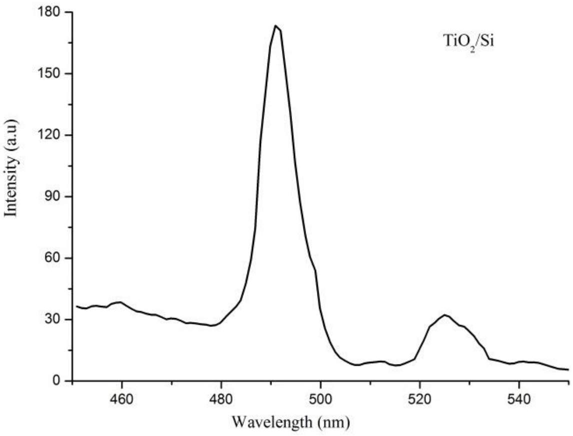

Figure 3 PL spectra of the TiO_2/Si structure

FTIR analysis

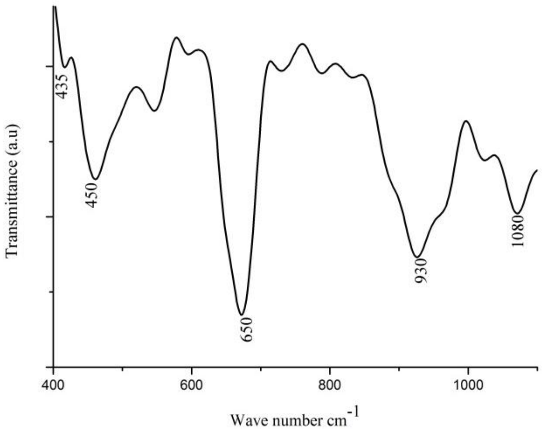

Figure 4 FTIR spectra of TiO_2/Si structure

Figure 4 shows the FTIR transmission spectrumof TiO_2 thin film coated Si. The bands at 435 cm^{-1}, 450 cm^{-1}, 650 cm^{-1}, 930 cm^{-1} and 1080 cm^{-1} are observed in the FTIR spectrum. The bands at 435 $cm^{-1}$and 650 cm^{-1} wereattributed to Ti-O stretching and Ti-O-Ti bending respectivelyfor TiO_2 crystalline structure. The asymmetric Si-O-Sirocking and stretching vibration modes were observed respectively at 450 cm^{-1} and 1080 cm^{-1}. The band at 930 cm^{-1}arises from Ti-O-Si stretching mode[6].

Conclusion

TiO_2 thin films have been deposited on silicon substrate by sol–gel process using spin coating technique. The XRD pattern of TiO_2/Si contains silicon peak along with anatase and rutile phases of TiO_2. The calculated crystallite size was found to be 32 nm. The percentage of anatase and rutile phases of TiO_2/Si was also found. The emission peaks at 485 nm and 530 nm are observed in the PL spectrum.The peaks are due to oxygen vacancies and impurities& defects. SEM image shows the non-homogeneous mosaic like structure. The presence of Ti, O and Si elements was confirmed from EDAX studies.FTIR analysis shows the presence of Ti-O-Si bond at 930 cm^{-1}. From the present study it could be concluded that *n*-TiO_2/*p*-Si structure can be probably used for sensor and solar cell applications.

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