Report of Major Research Project
No.F/39-503/2010(SR)04-01-2011
A study of the effect of doping of TiO_2 thin films with Fe and N on the structural, optical, photocatalytic and band gap narrowing properties.
carried out by **Dr. P.V.Thomas, Principal Investigator**
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Brief report of the work done

1. Preparation of pure TiO2 thin films in anatase phase.

TiO_2 thin films were prepared by RF magnetron sputtering. The procedure require high purity sputtering target and clean quartz substrates. Optimization of various sputtering parameters viz. sputtering pressure, sputtering time, Ar:O_2 ratio, substrate temperature and post deposition annealing temperature was done to obtain high quality TiO_2 thin film in anatase phase. The prepared films were annealed at 773, 873, 1073 and 1273 K for 2 h in air/oxygen atmosphere and characterised by XRD, Micro Raman Spectroscopy, XPS, SEM, UV-Vis spectrophotometry and PL studies.

TiO_2 films deposited at substrate temperature 573 K. sputtering pressure 0.01 m bar, RF power 300 W in pure Ar atmosphere and annealed at 873 K for 2 h exhibited better crystallization to anatase phase. Also optical properties, refractive index and band gap were tuned in this method by varying sputtering parameters.

2. Photocatalytic activity of pure and Fe doped TiO_2 thin films

TiO_2 is desirable as a photocatalyst due to its low cost, strong oxidising properties and non toxicity and photo-stability.

To photo activate TiO_2 UV light has to be used. Solar light has only 3-4% UV light. Reduction in the band gap of TiO_2 (band gap narrowing) is required for its photo activity in the visible region. This was achieved by doping TiO_2 thin film with Fe. Ionic radius of Fe^{3+} (0.064 nm) is identical to that Ti^{4+} (0.06 nm) and can easily substitute the crystal lattice of TiO_2

Experimental details:

Two methods were used in this study to dope TiO_2 films with Fe^{3+}.

(a) Homogeneous doping

Standard ceramic procedure was used to prepare sputtering targets. High purity Fe_2O_3 powder was used as the dopant. Atomic ratios Fe/Ti were chosen as 0.02, 0.05, 0.10 and 0.50 at % for doping studies. It was concluded that TiO_2 film doped with 0.15 at % showed better crystallinity to anatase structure suitable for photocatalytic activity.

(b) Non homogeneous doping

In this method Fe_2O_3 pellets (thickness 3mm, diameter 1 cm) were placed on top of TiO_2 ceramic targets. The percentage of Fe in sputtered films was varied by placing Fe_2O_3 pellets at different positions on erosion ring of the TiO_2 target.

It was observed that non homogeneous doping resulted in appreciable reduction in band gap of TiO_2 (band gap narrowing). This has helped to achieve better photocatalytic property when solar light is used to irradiate Fe doped TiO_2 thin films. The detailed study was done and appreciable result was obtained. Non homogenous doping resulted in better reduction of band gap.

To verify the effect of Fe doping, to enhance photocatalytic property of TiO_2 films, we did studies on the degradation of Methylene Blue (MB) by deposited TiO_2-Fe thin films in UV light (from high pressure Hg lamp) and sunlight.

Non homogenously doped TiO_2 exhibited enhanced photocatalytic activity (77.47%) compared to homogeneously doped TiO_2 films (69.37%).

We found that doped Fe-TiO_2 Films exhibited high photocatalytic activity. The details of the studies and results are given in the papers published.

The studies can be extended to N doped TiO_2 thin films.

Details of the Project

Major Research project	:	No. F/39-503/2010 (SR) 04-01-2011
Principal Investigator	:	Dr. P.V. Thomas
Tenure of the project	:	3 years from 1-2-2011 to 31-1-2014
Grant Received	:	Rs. 512800/-
No of papers published	:	5
No. of PhD awarded`	:	1

Prabitha B Nair (Project fellow), PhD awarded by University of Kerala (2013)
Title : A study on the structural, optical, photoluminescence and photocatalytic properties of pure TiO_2 and M doped (M=Fe, Tb) TiO_2 thin films prepared by RF Magnetron sputtering.

Papers published from 2011-2014 under this Project

1. Effect of RF power and sputtering pressure on the structural and optical properties TiO_2 thin films prepared by RF magnetron sputtering
Prabitha B.Nair[a,1], V.B. Justinvictor [a-2] Georgi P. Daniel [a-3] K. Joy[a-4] ,
V. Ramakrishnan [b-5] P.V. Thomas [a*]
Applied Surface Science 257 (2011) 10869-10875

2. Influence of film thickness and annealing atmosphere on the structural, optical and luminescence properties of nanocrystalline TiO_2 thin films prepared by RF magnetron sputtering.
Prabitha B. Nair, V.B. Justinvictor, Georgi P. Daniel, K. Joy P.V. Thomas
J.Mater.Sci.Mater Electron (2013) 24:2453-2460

3. Structural, optical, photoluminescence and photocatalytic investigations on Fe doped TiO_2 thin films
Prabitha B.Nair, [a]V.B. Justinvictor[a], Georgi P. Daniel[a], K.Joy[a],
V.Ramakrishnan[b], David Devaraj Kumar [c], P.V. Thomas [a]
Thin solid films 550(2014) 121-127

4. Investigations on the structural and optical properties of RF magnetron sputtered TiO_2 thin films: effect of substrate temperature and $Ar:O_2$ ratio.
Prabitha B. Nair, V.B. Justinvictor , Georgi P. Daniel , K.Joy , K.C. James Raju, P.V. Thomas [a]
Journal of optoelectronics and advanced materials Vol. 16,no. 3-4 p.360-369 (2014)

5. Optical parameters induced by phase transformation in RF magnetron sputtered nanostructured TiO_2 thin films
Prabitha B. Nair, V.B. Justinvictor , Georgi P. Daniel , K.Joy , K.C. James Raju, David Devaraj Kumar, P.V. Thomas[a*]
Progress in Natural Science Materials International 24 (2014) 218-225.