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Synthesis of Titaniumdioxide (TIO_2) Nano Particles

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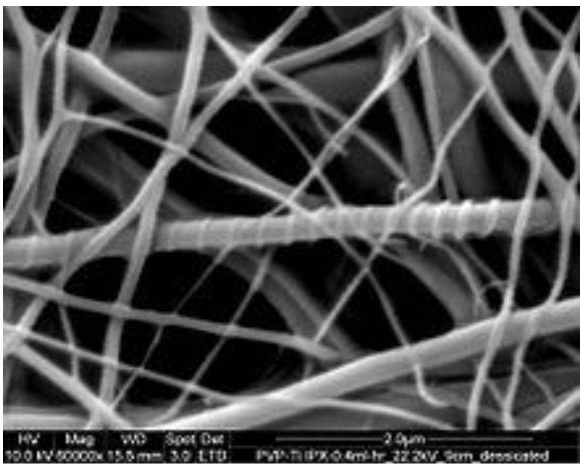
Abstract: *Titanium dioxide nano particles (TIO_2) were prepared by sol-gel technique. The synthesised nanoparticles were characterised for their structure using XRD, SEM and FTIR. Debye scherrer powder technique was used for calculating the average size of the sample. Surface morphology was estimated using SEM. Band gap = 3.2 eV.*

Keywords: *Titanium dioxide, Sol-gel technique, XRD, Debye-scherrer technique.*

I. Introduction:

Titanium dioxide is a photo catalyst once illuminated by light with energy higher than its band gaps, electrons in Titanium dioxide (TIO_2) will jump from valence band to conduction band. Electron hole pairs were formed on the surface of photo catalyst. The negative electrons and O_2 will combine O^{2-} and positive electric holes and H_2O will generate hydroxyl radicals. Since both are unstable it will combine with O^{2-} and OH^- respectively and turn into carbondioxide and water. This cascade reaction was formed when an organic compound falls on the surface of photo catalyst. Titanium dioxide (TIO_2) mainly exists in three crystalline forms such as anatase, rutile and brookite. The three crystal structures consist of TIO_2 octahedron connected variously by corners and edges. This work was focussed on synthesis of anatase TIO_2 nano particles by sol-gel method.

Titanium dioxide particularly in anatase form, is a photo catalyst under ultra violet (UV) light. Titanium dioxide when doped with nitrogen ions or doped with metal oxide like tungsten trioxide is also a photocatalyst under either visible light or uv light. The strong oxidative potential of the positive holes oxidises water to create hydroxyl radicals. It can also oxidise oxygen or organic materials directly.



1.1 Crystal Structure Data Of Tio_2

Property	Rutile	Anatase	Brookite
Crystal structure	Tetragonal	Tetragonal	Orthorhombic
Lattice Constant	a= 4.5936 c=2.9587	a=3.784 c=9.515	a=9.184 b=5.447 c=5.154
Molecule (Cell)	2	2	4
Volume / mol (A3)	31.2160	34.061	32.172
Density (g cm^{-3})	4.13	3.79	3.99
Ti – O Bond length	1.949 1.980	1.937 1.965	1.87- 2.04
O – Ti – O Bond angle	81.2 90.0	77.7 92.6	77.0 - 105

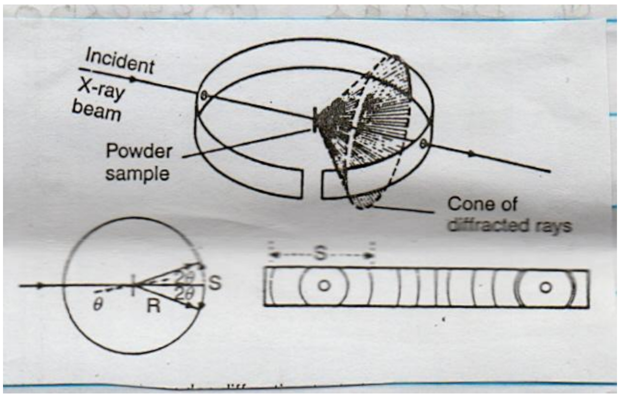
II. Experiment

2.1 Preparation of TiO_2 Nano particles by sol-gel method.

Titanium dioxide nano particles in 5nm range were prepared by sol-gel method. The titanium dioxide nano particles prepared were calcinated at 450 C. The sample contained 72.4% of anatase and 27.6% weight in amorphous phase. The synthesised product was obtained from Titanium (IV) iso propoxide dissolved in ethanol. Certain amount of deionised water was added to the solution in molar ratio of Ti: H_2O = 1:4. The mixed solution was vigorously stirred for 1 hour in order to form sols. The sols were transformed into gel after a day. The gels were dried at 120 C to remove H_2O for one day. Now the dried gel was sintered at 450 C for 2 hours in high temperature furnace. Finally the pure TIO_2 nano particles were obtained.

2.2 Debye – Scherrer method

A monochromatic X-ray beam was incident on a powder sample contained in a fine walled glass tube. The tube was rotated to smooth out the recorded diffraction pattern. The conical pattern of X rays emerging for each angle 2 O with O satisfying the bragg condition was incident on film strip in arcs. Bragg angle has the value O=s/4R where s is the distance between two corresponding reflections on film and R is the radius of film. Thus a single exposure of powder to X ray beam provides all bragg angles at the same time. This technique is used for sample identification.



III. Results And Discussion

3.1 X RD

X – Ray diffraction pattern gives information about crystalline structure, grain size and lattice strain.

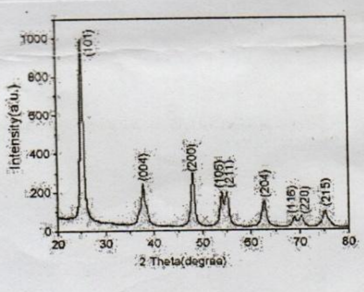
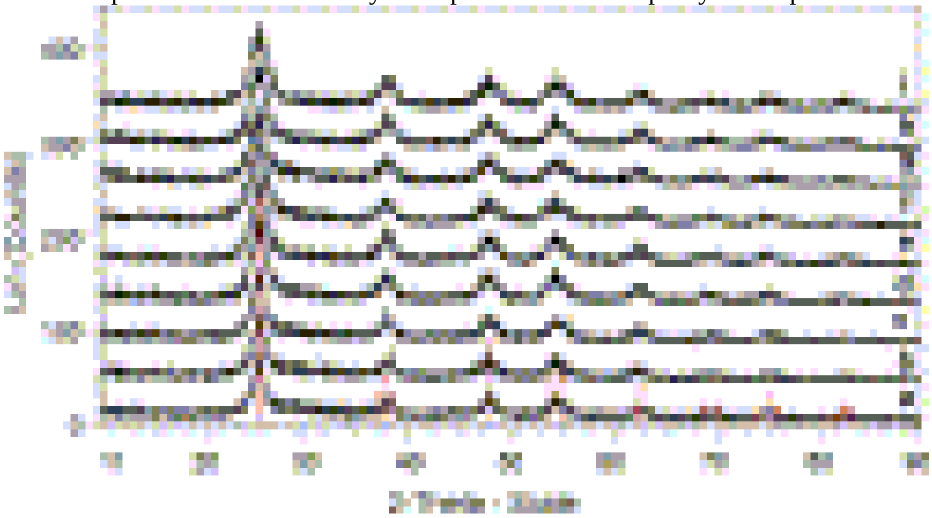


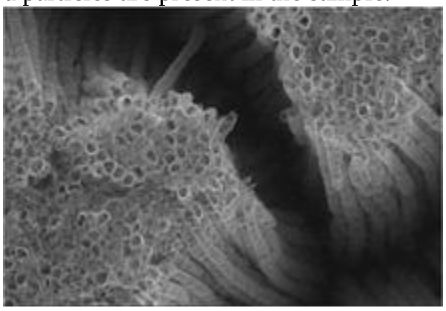
Fig. 1. X-ray diffraction of prepared TiO_2 nanoparticles.

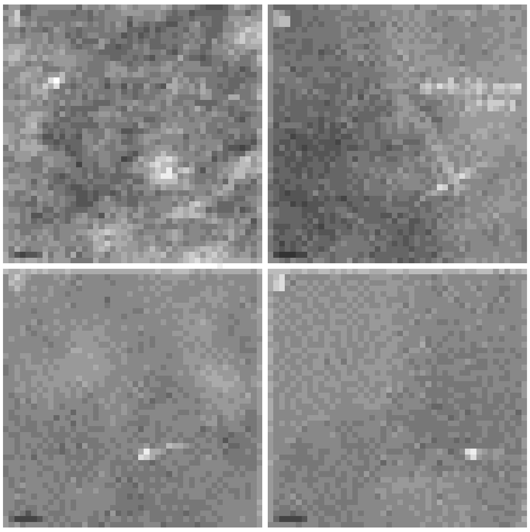
Fig shows the XRD pattern of synthesised TIO_2 nanoparticles calcinated at 450 C. All the diffraction peaks of the samples are indexed well to tetragonal anatase, crystalline phase of TIO_2. The presence of peaks corresponds to anatase phase and absence of any other peak confirms the purity of sample.

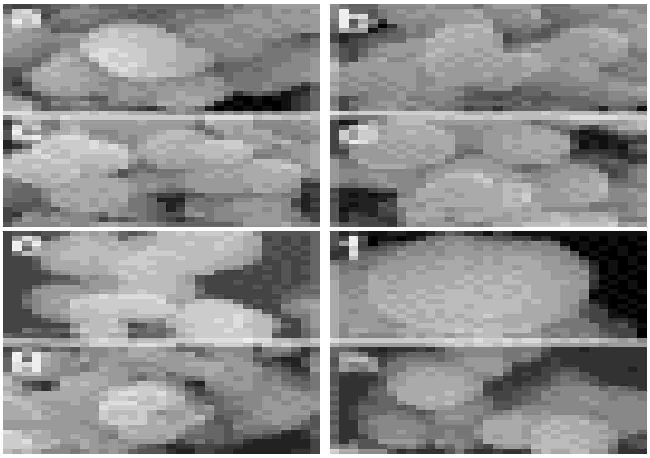


3.2 SEM

The grains have uniform shape and large agglomeration which occurs in the form of cluster. SEM images are shown below. More spherical shaped particles are present in the sample.







3.3 FTIR

Between 450 and 800 cm^{-1} is the characteristic mode of TIO_2. The absorbance range around 3429 cm^{-1} indicates the presence of hydroxyl. The absorption range around 1636 cm^{-1} indicates hydroxyl (bending) groups of molecular water.

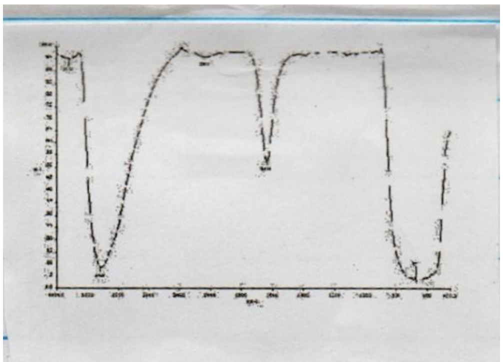


Fig. 4. FTIR spectrum of prepared pure TiO_2 nanoparticles.

IV. Conclusion

The prepared anatase of TIO_2 nano particles can be used for applications like dye sensitised solar cells. The SEM observation clearly reveals that the particles are strongly aggregated and appeared in porous morphology. The SEM images show a good crystalline nature. Nano scaled titanium dioxide particles are used in sun screen lotion because they scatter visible light. Its strong uv light absorbing capabilities and its resistance to discolouration under ultraviolet light enhances its stability.TIO_2 is considered very close to an ideal semi conductor for photo catalysts because of high stabililty and safety towards human and environment.

Synthetic single crystals of TiO_2, ca. 2–3 mm in size, cut from a larger plate.

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