Chapter VII

Conclusions and Future Scope

The important findings of the thesis were outlined below:

- In this thesis, TiO_2 nanoparticles were synthesized through simple, cost effective sol-gel technique and were examined for its structure, microstructure as well as photocatalytic properties under UV light and sunlight. Additionally, the biocompatibility of TiO_2 nanoparticles was investigated. TiO_2 nanoparticles of crystallite size 33 nm were stabilized with anatase phase. Photocatalytic study of the TiO_2 nanoparticles were undertaken by examining the degradation behavior of most common organic dyes such as MB, CR and RhB after illuminating with UV light as well as sunlight. We found that 100% degradation of MB and RhB after 180 min, whereas, CR degraded after 120 min under UV-irradiation. However, under sunlight, the photocatalytic degradation of the dyes, MB, CR and RhB with TiO_2 nanoparticles took, 90, 45 and 180 min**,** respectively. Further, we studied the biocompatibility of TiO_2 nanoparticles and observed hemocompatible nature, no platelet aggregation and no significant change in ROS. We concluded that these TiO_2 nanoparticles were found to be an efficient photocatalyst under sunlight as well as biocompatible in nature. These TiO_2 nanoparticles can be employed as an active photocatalytic material for purification of industrial effluents.
- Since TiO_2 was exhibited good photocatalytic degradation behavior with different dyes under sunlight, for its potential use, we fabricated TiO_2 and cement composite pellets of three different compositions, named as TC1, TC2, TC3 and

studied its photocatalytic properties in the presence of sunlight. A single pellet of TC1 containing 50 mg of TiO_2 degraded ~100% of CR and MB within 120 min of irradiation. On the other hand, four pellets of TC2 and TC3 with 20 and 10 mg of TiO_2 and 50 mg of cement, showed ~85-100% degradation of CR and MB after 240 min of irradiation. TC1, although revealed a high photocatalytic performance, but due to less stability of the pellet we could not use it repeatedly. Therefore, we concluded that composites of low TiO_2 content i.e. TC2 and TC3 which were cost effective and were found to be used efficiently for industrial waste water purification.

- Structural, magnetic, photocatalytic and antibacterial properties of TiO_2 nanoparticles were studied after doping 1 to 3 at% of Mn. While XRD patterns showed the mixed phase of anatase and rutile for 1 and 2 at% of Mn, 3 at% of Mn doped TiO_2 exhibited pure anatase phase. Such phase transformation from mixed anatase and rutile phase to anatase one with increasing Mn concentration was not reported earlier. The particle size of 1 and 3 at% doped sample was 15 and 12 nm estimated from TEM, respectively, were of single crystalline nature observed from SAED patterns. We revealed that the particles of 12 nm stabilized the anatase phase in 3 at% of Mn doped TiO_2. From XPS, it was observed that oxygen vacancies present in both 1 and 3 at% Mn doped samples were accompanied with various oxidation states of Ti and Mn. As a result, we observed a ferromagnetic behavior at 10 K. First time, we successfully demonstrated 100% photocatalytic degradation of CR and more than 80% degradation of MB in 1 h

using only 20 mg of Mn doped TiO_2 under sunlight irradiation. Besides catalytic behaviour, Mn doped TiO_2 samples also exhibited the antibacterial property.

- TiO_2 thin films deposited through e-beam evaporation technique and annealed at 500 and 900 ºC were irradiated with 500 keV Ar ion. Under irradiation, the evolution of structure, surface morphology and magnetic properties of TiO_2 thin films were discussed. It was observed that film annealed at 500 ºC crystallized in anatase phase. After irradiating with ion fluence in the range of 1×10^{14} to 1×10^{16} ions/cm^2, crystalline film transformed to amorphous phase. When the film was irradiated with 5×10^{16} ions/cm^2, crystalline behavior was revived and phase was found to be brookite. Although anatase to rutile phase transformation is an usual phenomenon, the transformation from anatase to brookite phase through intermediate amorphous phase was observed for the first time in TiO_2 thin films under irradiation. Magnetic measurements showed RTFM irrespective of phase and crystallinity. The unusually high saturation magnetization in amorphous films than in crystalline ones was explained on the basis of higher oxygen vacancies confirmed from XPS.
- TiO_2 thin films annealed at 900 ºC, after 500 keV Ar^{2+} ions irradiation, showed phase transformation from anatase to brookite phase. Moreover, an impurity phase, Ti_4O_7 was observed in pristine as well as in irradiated films indicating a radiation resistant behavior. From AFM, it was found that roughness was more in pristine film than in the irradiated films. Magnetic measurements showed RTFM irrespective of phase and crystallinity. Higher saturation magnetization in pristine

film than in irradiated ones could be due to higher oxygen vacancies, obtained from XPS.

Our investigations on nanoparticles and thin films of TiO_2 revealed several new and important findings. However, there are several open issues which need to be clarified with proper experimentation. Few important suggestions for future work are appended below.

- Photocatalytic degradation of other organic impurities under sunlight can be studied as the photocatalytic activity of TiO_2 nanoparticles under sunlight for broad use.
- Structure and surface morphology of pristine and irradiated TiO_2 thin films of different thickness can be studied after irradiating with low energy ions of different ion fluence.