Executive summary of the project

Title of the project: Photocatalysis using nanocrystalline titania

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Tenure of the Project: 18 months

Total Grant Allocated: 1,65,000

Total Grant Received: 1,59,500

Objectives of the project:

The objectives of the project were to synthesize TiO_2 nanoparticles with particle sizes ranging between 2 and 20 nm, and to study the photocatalytic activity of the nanoparticles. The proposed studies included synthesis, characterization, and application of TiO_2 nanoparticles as photocatalyst in the visible range. The first part of the proposed work was to synthesize anatase which absorbs in the visible range and then to study its photocatalytic activities. It was planned to synthesize titania with high surface area in the anatase phase form and also with controlled phase composition by controlling the processing parameters.

Summary of the work:

Titanium dioxide (TiO_2) is a well-known, wide-band-gap, n-type semiconductor oxide. TiO_2 forms three distinct polymorphs: rutile, anatase, and brookite. Photocatalysis using TiO_2 has been developed and continued to hold a dominant position in photocatalysis. Anatase and brookite have attracted a great deal of interest in connection with technological applications. Anatase plays a key role in the injection process of photochemical solar cells with high conversion efficiency. Recently, much attention has been focused on the photocatalytic properties of TiO_2, which has good stability in the outdoor environment, for the purification of environmental air and water samples, deodorization, and antibacterial and self-cleaning coatings. However, because of its high-energy band gap (3.2 eV for the anatase form) TiO_2 can harvest only a small fraction (less than 5%) of incident solar energy. Therefore, in order for it to be used outdoors, a TiO_2 photocatalyst must respond to visible light with better efficiency, since 45% of the energy in sunlight is in the visible region. To attain efficient visible light-active TiO_2, it is important to extend its absorption spectrum into the visible range.

TiO_2 can be used as a photocatalyst for the removal of highly toxic and non-biodegradable pollutants normally present in air and wastewater via photocatalysis, which is a low temperature, non-energy intensive process for the chemical waste remediation. TiO_2 has been the photocatalyst of choice due to its photostability, non-toxicity, redox efficiency and availability. Being more photocatalytically active, chemically stable, environmentally friendly, and cheaper TiO_2 has been the most promising one for the photocatalysis compared to other semiconductors. TiO_2 nanoparticles offer additional advantages if the size can be optimized. The material properties of TiO_2 nanoparticles are a function of the crystal structure, nanoparticle size, and morphology and, hence, are strongly dependent on the method of synthesis. In photocatalysis research, anatase titania is usually considered to be more active than crystalline rutile. Generally, among the various phases of titania reported, anatase shows a better photocatalytic activity.

Titania nanoparticles of size ~5 nm were synthesized by a simple method using titanium isopropoxide. The nanoparticles were characterized by different techniques such as powder X-ray diffraction, TEM, UV-Visible and IR spectroscopy. X-ray diffraction studies indicated the formation of the anatase phase of titania in the as-synthesized powder. The sizes of the nanoparticles were increased up to 30 nm, with increased crystallinity, by calcination of the as-synthesized powder at different temperatures.

Photocatalytic activity of the synthesized titania nanoparticles was studied using the photodegradation of methylene blue dye. From the studies using titania particles of three different sizes (5 nm, 10 nm, 30 nm), it was found that the catalytic activity increases with increasing particle size. The photocatalytic decomposition of methylene blue was found to follow first order kinetics. However, from powder X-ray diffraction studies on the powders calcined at 400 and 600 ^{o}C, it was also observed that part of the anatase phase is converted to the rutile phase and the rutile phase content increased with increasing calcination temperature. Therefore, from the results, it has been concluded that the increased photocatalytic activity of the calcined powders is due to the combined effect of increasing crystallinity of the anatase phase as well as the presence of rutile phase in the powders.

The present study showed that titania nanoparticles can be prepared in the anatase phase by a simple solution based chemical process and the light absorption region of anatase phase of titania can be extended to the visible region by changing the processing conditions. Photocatalytic activity of the nanocrystalline titania is studied by following the decomposition of methylene blue dye. From the studies on three different samples with increasing particle size as well as increasing rutile phase content, it was found that the photocatalytic activity increases with increasing the rutile phase content. However, the contribution of the increasing crystallinity of the anatase phase with increasing particle size cannot be ruled out because the as-synthesized sample without any rutile phase also showed sufficient photocatalytic activity. Further studies are planned to understand the effect of the role of crystallinity, particle size and rutile phase on the photocatalytic activity of nanocrystalline titania.