Structure and Physical properties of TiO_2

Titanium dioxide (TiO_2) is highly important in both theoretical and experimental field of research because of its very interesting electronic structures and wide band gap (3.2 eV for anatase) which can be tuned by several processes. It has wide range of industrial and technological applications as pigment, photo catalyst and UV absorption. Hence, TiO_2 is an important compound suitable for fuel cells, solar cells, different sensors, pollution control system, waste management and self-cleaning glass coating materials along with food, cosmetic, paint, UV protector etc. Nontoxicity, chemical stability, poor solubility and high refractive index are properties which add to its practical applicability. TiO_2 has mainly three crystal structure: anatase (tetragonal, space group I41/amd), rutile (tetragonal, space group P42/mnm) and brookite (orthorhombic, space group Pbca). Rutile phase formation starts above 600 °C while anatase forms at lower temperature. At a lower synthesis temperature (600 °C), TiO_2 nanoparticle tends to nucleate to an anatase phase as surface Gibbs free energy is lower for anatase phase than the rutile.

Physical properties of TiO_2 not only depend on the phase structure but it depends also on the agglomerated micro structure, pores and particle size. For different physical and chemical process like charge transfer, chemical reaction, photon absorption etc. the molecules on the surface of a particles are more active than those stay inside. Hence surface offers more efficiency and TiO_2 nanoparticles with higher surface to volume ratio become extremely favorable from the application point of view.

The aim of our work is to observe the effect of different parameters (like heating/cooling rate, calcination time, environment, pressure, pH, dopants etc.) on phase transition, grain growth process, surface morphology, properties etc..