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Synthesis and characterization of TiO2: Evaluation for possible application as light trapping layer in thin film solar cells.

In this study, titanium dioxide (TiO_2) nanoparticles were synthesized using the sol–gel method, setting the reaction time at 2, 4, and 6 h. The synthesized samples were then annealed at 500℃ for 3 h. Structural, morphological, compositional, and optical characterization was carried out using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) coupled with energy-dispersive X-ray (EDX) spectroscopy, and UV-VIS spectroscopy. The XRD patterns confirmed the crystalline nature and tetragonal structure of the TiO_2 nanoparticles, while the average grain size and dislocation line density were also estimated using the Debye–Scherrer relation. The Anatase (2 hr and 6 hr samples) and rutile (4 hr sample) phases were confirmed, and the average crystallite size was found to be 4.75 nm for the sample prepared at 2 hrs, 27.24 nm for 4 hrs, and 4.38 nm for 6 hr reaction time. The crystallite size for the 2-hr sample decreased from 4.75 nm before annealing to 3.69 nm after annealing, while the dislocation density increased from 0.01 × 10^{15} to 0.245 × 10^{15} lines/m^2. A significant reduction in crystallite size was also observed in the 4-hr sample. Before annealing, the crystallite size of the 4-hr sample was 27.24 nm, which significantly dropped to 3.97 nm after annealing, accompanied by a decrease in dislocation density from 0.484 × 10^{15} to 0.108 × 10^{15} lines/m^2.Moreover the crystallite size for the 6-hr sample decreased from 4.38 nm before annealing to 3.72 nm after annealing, while the dislocation density increased from 0.770×10^{1}5 to 1.125×10^{1}5 lines/m^2. FTIR identified the functional groups comprising O–H (broad band around 3400 cm^{-1}), H–O–H bending (1620 cm^{-1}), and Ti–O/Ti–O–Ti stretching vibrations (in the range of 500–700 cm^{-1}). Raman spectroscopy further validated the presence of anatase and rutile phases through peak analysis .The presence of sharp and intense Raman peaks, particularly for the anatase samples, indicates improved crystallinity and reduced structural disorder after annealing. SEM analysis showed that longer stirring times (2–6 h) and subsequent annealing led to increased grain size, better particle uniformity, and enhanced crystallinity with reduced porosity. EDS analysis confirmed the elemental composition of TiO_2 with high purity, showing predominant peaks for titanium and oxygen. The UV-Vis spectra showed absorption at approximately 390 nm for the 2 hr and 6 hr samples, corresponding to the anatase phase, and around 420 nm for the 4 hr sample, indicating the rutile phase.The samples prepared with 2hr and 6hr reaction times, exhibited a relatively improved absorption. This study is conducted to fine-tune and optimize the properties of TiO_2 nanoparticles for potential applications in photovoltaics, such as perovskite-based solar cells.

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Primary author: Ms JAFFAR, Rida (University of south Africa)

Co-authors: Prof. MATHEVULA, Langutani (University of south Africa); Prof. PONTSHO, Mbule (university of south Africa)

Presenter: Ms JAFFAR, Rida (University of south Africa)

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