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Study of the Structure and Optical Properties of *TiO2* Prepared via Pulsed Laser Ablation for Photocatalytic Applications

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The nanodispersed titanium dioxide is currently widely used in photovoltaic devices that find application in the green solar energy technologies, as well as in production of bactericidal materials and sunscreen creams. However, it is the heterogeneous photocatalysis that holds the most promise as a field of its application.

Currently, new technologies to synthesize titania-based materials, which absorb light in the visible region and have high photocatalytic activity, are developed. Pulsed laser ablation (PLA) has attracted a great interest, since this technique allows obtaining pure nanocolloids and nanocrystalline powders during ablation in liquids or vacuum or gaseous media. Despite a lot of research, there is not enough knowledge about structure and properties of the titanium dioxide synthesized by PLA method. This is due to the difficulties associated with obtaining a sufficient amount of ultrafine powder for research.

TiO2 powder were synthesized using Nd:YAG laser (wavelength of 1064 nm, frequency of 20 Hz, pulse duration of 7 ns). Some of the samples were annealed at temperatures of 100 - 1000 °C.

The initial TiO2 is a dark blue powder consisted of spherical crystallites with an average size of 5-10 nm and an insignificant number of large particles with a size of up to 80 nm. After annealing the sample changes color to light grey at 400°C and becomes white at 600°C. According to XRD data and Raman spectroscopy, the material is nanocrystalline and consists of phases of anatase and rutile. Also it should be noted that this method of preparation allows obtaining nanoparticles with anatase phase more resistant to temperature effects.

X-ray photoelectron spectroscopy data shows that only the doublet with bond energy of 458.5 eV (Ti2p3/2) corresponding to Ti^{4+} state. Photoemission spectra from level O1s with subsequent deconvolution gives two peaks with bond energies 529.7 eV which corresponds to lattice oxygen of titanium dioxide and 531.9 eV belongs to adsorbed oxygen on the surface of titanium dioxide.

It was found that TiO2 diffuse reflection spectra had an intense additional absorption in visible region. This additional absorption is due to the presence of defects of various nature in the structure of TiO2, namely, different types of oxygen vacancies. (F, F^{+} and F^{2+}-centers). These F^{+} and F^{2+} defect states can act as traps captured photoexcited electrons, that increases the charge carriers lifetime and prevents their recombination [1]. It was found that with an annealing temperature increase, the number of defective states decreases. This affects the absorbtion intensity in the visible region, and also affects the color of the samples. The calculated band gap was 2.65 eV. Decrease in the band gap value is due to the presence of defect levels in the band gap that lie higher in terms of energy than 2pO levels forming the valance band of TiO2. Therefore, the defect levels blur the clear boundary of the valance band, and they appear as additional absorption in the visible spectrum. It was found that with an annealing temperature increase, the number of defective states decreases. This affects the absorption intensity in the visible region, and also affects the color of the samples.

Thus, by pulsed laser ablation, we have prepared nanocrystalline titanium dioxide witch absorbs intensively in the visible range of spectrum, and can be used for photocatalytic applications.

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References

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