Physico-Chemical nanomaterials science

Modification of nano-sized barium titanate and its catalytic properties

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Barium titanate (BT) is traditional electroceramic material. At the same time, BT as wide-gap semiconductor possesses photocatalytic properties. Among other things, the efficiency of BT use is determined by its dispersion (specific surface area SSA), presence of structural (intrinsic) defects and impurities (extrinsic defects). We used dry ball-milling for synthesis, activation and doping of BT with transition metals in order to improve its photocatalytic properties. The latter were evaluated *via* dyes degradation in aqueous media.

In the first case, BT with SSA=7 m^2/g, which was prepared by traditional solid state procedure, was used as initial and reference material. This BT is active only under UV-illumination since band gap Eg=3.10 eV. Its ball-milling leads to increase in SSA value 2 times and generation of crystal structure defects. This is accompanied by increase of visible light absorption and narrowing of band gap to 2.90 eV. As a result, the rate constant of dye degradation K_d, as photocatalytic activity measure, also increases 2-3 times under UV-irradiation. In addition, more importantly, milled BT acquires the activity under the influence of visible light. An even greater effect was obtained by using BT doped with Zn and Fe. Thus, the doping results in reduction of E_g value to 2.75-2.80 eV and increase of photocatalytic activity under visible irradiation: K_d reaches the magnitudes $(4.4\text{-}6.1)\cdot10^{-5}$ s^{-1} even in the process of degradation of such a stable dye as safranin T. In the second case, direct mechanochemical synthesis of BT with SSA=25-65 m^2/g (and crystallite size – 15-30 nm) from barium and titanium oxides was realized. The next thermal treatment of all milled sample leads to defects relaxation, which is confirmed by ESR and XPS measurements, and the band gap value increases. It has been established linear relationships between photocatalytic activity of BT samples and values of their specific surface area (direct-proportional) band gap (inverse-proportional).