Precursor influence on the granulometric and optical properties of flame made titania

M. Stanzel[1], M. Domaschke[1] and W. Peukert[1,2]

[1]Institute of Particle Technology, Friedrich-Alexander-University Erlangen-Nuremberg, Cauerstr. 4, 91058 Erlangen, Germany
[2]Interdisciplinary Center for Engineering of Advanced Materials (EAM), Friedrich-Alexander-University Erlangen-Nuremberg, Nägelsbachstr. 49b, 91052 Erlangen, Germany

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Presenting author email: melanie.stanzel@fau.de

Nanoparticulate titania is, due to its high refraction index, mainly used as a nontoxic and economic white pigment in paintings and lacquers to improve their coverage and tint reducing power. As a wide band gap semiconductor and photocatalyst it is, dispersed in organic solvents and deposited as thin film on e.g. flexible substrates, also applied in printable electronic devices, such as DSSCs or catalysts for self-cleaning. (Chang et al., 2008)

To cover the high demand of this low cost material an energy efficient and solvent free synthesis method with high production rates, for example a flame spray process, is required. Utilizing this technique particle size, shape, optical band gap and defect states of the particles can be controlled by the formulation of the precursor and the synthesis route. In this work, a systematic study about the usage of different titanium precursor salts and various solvents is conducted. The resulting particles are successively analysed regarding their optical and morphological properties. Especially, the influence of solvent boiling point and combustion enthalpy as well as the molar weight of the salt are taken into account.

Different liquid precursors, Ti-isopropoxide, Ti-2-ethoxide, Ti-2-ethylhexyloxide and Ti-2-ethylhexanoate dissolved in various solvents, are dispersed by a nozzle into the spray flame. In the flame, pyrolysis reactions lead to high supersaturation and therefore to particle nucleation with subsequent growth, agglomeration and sintering. The solvent combustion enthalpy and boiling point are important set screws to tailor TiO_2 with desired properties. The reactor set-up (Siriwong et al., 2009) allows producing TiO_2 with different anatase and rutile phase composition and particle sizes in the range of 6 nm up to 60 nm. These particles are then collected on a membrane filter.

XRD measurements reveal the presence of two different titania phases, anatase and rutile. The non-gaussian peak shape, see figure 1, indicates a crystallite size distribution for anatase particles in a range of 6 nm to 60 nm. Figure 1 also indicates that structure equivalent salts lead to similar particle morphologies by using the same precursor solvent. The rutile phase shows a crystallite size, depending on precursor salt and solvent, between 15 nm and 40 nm. The composition of anatase and rutile can be influenced by either the combustion enthalpy or the type of salt. BET exhibits the specific surface and surface constitution of the TiO_2 nanopowders. Carbon contamination and surface attached species are determined via TGA and range from 4 wt% to 16 wt%. The optical bandgap measured by diffuse reflectance spectroscopy is linearly depending on the mass loss of the powders. Additionally, the photoluminescence characterizes defect states and oxygen vacancies, which are influenced by the solvent nature.

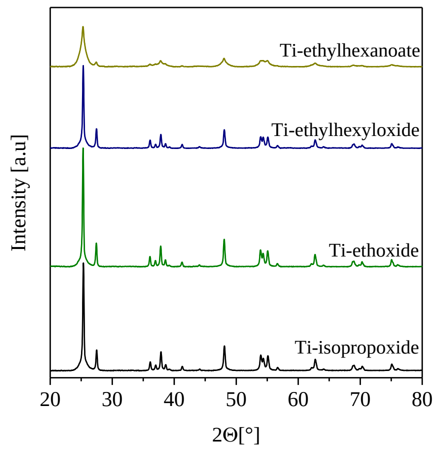

Figure 1. Diffragtograms of TiO_2 nanoparticles synthesized with different precursor salts in 2-methoxyethanol

The aerosol synthesis will be reviewed shortly. The properties of the titanium dioxide particles will be discussed regarding morphology, carbon content and opto-electronical properties. Special emphasis will be placed on the influence of the solvent boiling point, combustion enthalpy and molar mass of the precursor salt.

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