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BOOK OF ABSTRACTS

Chemical aspects of liquid-phase synthesis of titania nanocrystalline modifications

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Crystal modification of powder titania (anatase, rutile, brucite) of nanometer-scale particles have unique properties that are related to their catalytic and photocatalytic activity. A large number of publications and patents relating to new methods for TiO_2 producing based on sol-gel technology.

Recently tytanilchloride precursor was used for synthesis of oxide materials. It is obtained by mixing $TiCl_4$ with water at a temperature close to 0 °C. A substance obtained in this way conventionally denoted by the formula $TiOCl_2$. It does not correspond to real chemical composition of precursor because it does not take into account hydroxility of titanium atoms and the formation it aqua complex cations.

We found out that Ti^{4+} cations in the reaction medium formed $[Ti(OH_2)_6]^{3+}\cdot 3Cl^-$ complex compound with water molecules and Cl^- anions. The general reaction of titanium aqua complex formation can be written as an equation:

$$TiCl_4 + 6H_2O \rightarrow [Ti(OH_2)_6]^{3+} \cdot 3Cl^- + \frac{1}{2}Cl_2 . \quad (1)$$

However, chemical equilibrium in a solution at temperatures over 40 °C is disturbed as a result of the reaction:

$$Ti^{3+} + H_2O \rightarrow Ti(IV)OH + \frac{1}{2}H_2 \quad (2)$$

The resulting $[Ti(OH)(OH_2)_5]^{3+}$ cations subsequently change their chemical state, increasing the hydroxility degree of titanium atoms. This process is realized with the participation of water molecules contained in the core of the complex cations and Cl^- anions:

$$H_2O + Cl^- \rightarrow OH^- + HCl , \quad (3)$$

$$[Ti(OH)(OH_2)_5]^{3+} + OH^- \rightarrow [Ti(OH)_2(OH_2)_4]^{2+} + H_2O . \quad (4)$$

Thermally stimulated process of water dissociation (reaction 3) and increase in the hydroxility degree atoms of titanium precursor (reaction 4) leads to the formation of $Ti(OH)_4\cdot 2H_2O$ molecules, which provide the formation of TiO_2 nanoparticles at condensation. The rod-like rutile particles with diameter of 1÷3 nm and a length of 10÷40 nm are formed at a temperature of 40–80 °C in the acidic reaction medium (pH = 0,5÷2,0). For correction of chemical and charge state of precursor K_3PO_4 or Na_2SO_4 was added to its solution. Number of modifying additives in relation to $[Ti(OH_2)_6]^{3+}$ was 5 wt. %. The presence of PO_4^{3-}, SO_4^{2-} anions in the reaction medium dramatically changes the crystallization process and provides a formation of ellipsoidal anatase particle with size of 3÷5×4÷6 nm.

Features of formation of structure of nanocomposites of dipyridamole ether of diphenylolpropane and glucose

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Synthesis of new materials is energy intensive process. Because of this fact modification of existing widely used polymer is economically valuable. Polyepoxides and their oligomers are polymers that are constantly used as composite matrix. They yield on its ability to satisfy the demands of modern technologies only polyolefines and some representatives vinyl polymers. Intentions of multi-purpose using of epoxy composite materials stimulate the introduction in their composition of impurities. These impurities improve the heat resistance, wear resistance, chemical resistance, ability to protection from penetrating radiation and also perform the role of structural modifiers.

For work composite materials were received on basis of dipyridamole of ether diphenylolpropane, cured by triethylenetetramine in the ratio 1 : 0,18, and D – glucose (glucose monohydrate) with a particle size of 5. Mass concentration of glucose in the composition of polyepoxides amounted were 0,5; 1; 2; 10; 20; 30 and 50 %. Samples of initial components and obtained composite materials were investigated by the methods of scattering of X-ray radiation in large angles. Specific heat was investigated by the method of differential scanning calorimetry in the temperature range from 20 to 2000 °C.

Diffraction pattern of obtained composite allows to make the following conclusions: the chemical grid has amorphous structure and this structure is preserved until reaching the mass concentration of glucose 2 % in the composite material. The existencing of individual crystalline phase in the chemical structure of the grid appears as diffraction maximum at = 19. In the interval of concentrations of glucose 10–50 % separate inclusions crystalline phase merge and formcrystal structure, which similar to the structure of individual glucose. These resultes are consistent with research data of the specific heat of the parent compounds and epoxy composite materials and thermograms re-write these samples. It was established that the relaxation transitions disappear at repeated entries in the initial composite materials, in the area of 20–60 °C. So they can be explained of the presence of nedovrsenoj phase of epoxy resin, which share can reach 20 % without additional thermal action. Crystalline phase of glucose of epoxy composite material connected interaction with its reaction groups of polyepoxides matrix and hardener.