

**THE INTERNATIONAL SUMMER SCHOOL  
NANOTECHNOLOGY:**

**FROM FUNDAMENTAL RESEARCH  
TO INNOVATIONS**

**and**

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**BOOK OF ABSTRACTS**

### Chemical aspects of liquid-phase synthesis of titania nanocrystalline modifications

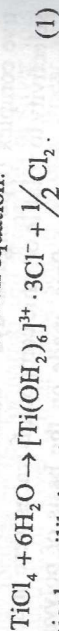
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Crystal modification of powder titania (anatase, rutile, brocrite) of nanometer-scale particles have unique properties that are related to their catalytic and photocatalytic activity. A large number of publications and patents relating to new methods for  $\text{TiO}_2$  producing based on sol-gel technology.

Recently titanilchloride precursor was used for synthesis of oxide materials. It is obtained by mixing  $\text{TiCl}_4$  with water at a temperature close to  $0^\circ\text{C}$ . A substance obtained in this way conventionally denoted by the formula  $\text{TiOCl}_2$ . It does not correspond to real chemical composition of precursor because it does not take into account hydroxylity of titanium atoms and the formation of aqua complex cations.

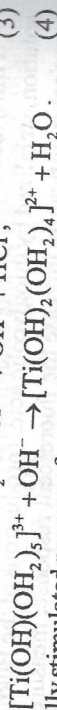
We found out that  $\text{Ti}^{4+}$  cations in the reaction medium formed  $[\text{Ti}(\text{OH})_6]^{3+}$ · $3\text{Cl}^-$  complex compound with water molecules and  $\text{Cl}^-$  anions. The general reaction of titanium aqua complex formation can be written as an equation:



However, chemical equilibrium in a solution at temperatures over  $40^\circ\text{C}$  is disturbed as a result of the reaction:



The resulting  $[\text{Ti}(\text{OH})(\text{OH})_2]^{3+}$  cations subsequently change their chemical state, increasing the hydroxylity degree of titanium atoms. This process is realized with the participation of water molecules contained in the core of the complex cations and  $\text{Cl}^-$  anions:



Thermally stimulated process of water dissociation (reaction 3) and increase in the hydroxylity degree atoms of titanium precursor (reaction 4) leads to the formation of  $[\text{Ti}(\text{OH})_4 \cdot 2\text{H}_2\text{O}]$  molecules, which provide the formation of  $\text{TiO}_2$  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  $40-80^\circ\text{C}$  in the acidic reaction medium ( $\text{pH} = 0.5-2.0$ ). For correction of chemical and charge state of precursor  $\text{K}_3\text{PO}_4$  or  $\text{Na}_2\text{SO}_4$  was added to its solution. Number of modifying additives in relation to  $[\text{Ti}(\text{OH})_6]^{3+}$  was 5 wt. %. The presence of  $\text{PO}_4^{3-}$ ,  $\text{SO}_4^{2-}$  anions in the reaction medium dramatically changes the crystallization process and provides a formation of ellipsoidal anatase particle with size of  $3-5 \times 4-6$  nm.

### Features of formation of structure of nanocomposites of dipyrindamole 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. Inventions 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 dipyrindamole 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  $2000^\circ\text{C}$ .

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 existing of individual crystalline phase in the composition of the grid appears as diffraction maximum at  $\theta = 19$ . In the interval of concentrations of glucose 10-50 % separate inclusions crystalline phase merge and form crystal structure, which similar to the structure of individual glucose. These results 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  $20-60^\circ\text{C}$ . 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.