PHASE FORMATION IN Ti-CuO SYSTEM UNDER REACTIVE SINTERING CONDITIONS [*]

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To date, combustion synthesis technologies as well as in the regime of reactive sintering have become widespread due to fundamental research. In particular, it is shown that if the physicochemical parameters of the medium, as well as the instantaneous spatial distributions of temperature and concentration are known, it is possible to calculate the reaction rate in the entire reactive mixture. Because of this, such processes are controllable and allow the synthesis of materials with desired structure and properties. It is known that if the rate of heat release from a reaction is lower than the rate of heat loss (e.g., due to conduction, convection), a self-sustaining process cannot be realized. This phenomenon is also key in bulk synthesis, as the self-propagating reaction can lead to inhomogeneities in the microstructure of the material, which is tried to avoid. The process should be made controllable. Liquid-phase sintering is one of the most promising methods of material synthesis today. About 90% of sintered materials are produced by this method.

In the present work we theoretically and experimentally analyze the process of bulk synthesis of composite from non-stoichiometric mixture of Ti and CuO powders, the simplified scheme of transformations in which can be represented as follows:

$$Ti+2CuO=TiO_2+2Cu;$$
$$xTi+yCu=Ti_xCu_y.$$
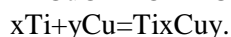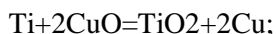
In the experiment, sintering is carried out both at temperatures below the melting points of the initial components and at temperatures leading to the appearance of the liquid phase. Preliminary studies have shown that the synthesis product has a non-equilibrium composition, and the reaction-diffusion interaction begins long before the melting of the reactants. The product contains a set of titanium oxides of different stoichiometry: TiO_2, Ti_2O_3 and TiO, as well as residues of depleted copper oxide Cu_2O. The set of intermeallide phases also turns out to be complex. The result is partly explained by the fact that partial decomposition of copper oxide starts long before the melting temperature of the oxide, and the metal particles (titanium) have an oxide film on their surface, which increases the energy barrier for metal-to-metal reactions. However, when the liquid phase is formed, the oxide film breaks and the liquid metal spread out to encompass the particle with a higher melting point, which increases the contact area and lowers the activation energy.

Taking into account the experimental data, a kinetic model in the null-dimensional approximation is proposed, taking into account the main physicochemical stages, as well as a number of modern approaches allowing determining the thermodynamic parameters of reactions are considered. As the basic equations of chemical kinetics, the Arrhenius law and the law of acting masses are used, which allow us to calculate instantaneous concentration distributions and trace the paths of formation of intermediate components. All assumed reaction pathways are based on literature data as well as on phase state diagrams.