PHYSICO-CHEMICAL MODELING OF THE PROCESSES OF OBTAINING POROUS GLASS COMPOSITE IN THE MARSHALITE-MICRO SILICON-NaOH SYSTEM

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Porous glass composites have specific properties: incombustibility, non-toxicity, environmental friendliness. Due to the combination of properties, porous glass composites are widely used in construction as heat insulators. Currently, two technologies have been developed for the synthesis of porous glass composites of the foam glass type: two-stage and one-stage technology. Onestage technology (alkaline technology) is less energy-consuming, simpler and cheaper. The essence of alkaline technology is the interaction of silica (SiO_2) with a solution of sodium hydroxide (NaOH). As a source of silica, the most promising is the use of natural raw materials. Currently, there is a trend to explore the possibility of using new types of natural raw materials. The scientific literature does not describe technologies for obtaining porous glass composite from marshalite with the addition of silica. In our work, for the first time, a glass composite was obtained from marshalite and microsilicon using a single-stage alkaline technology. As a result of the reaction between silicon dioxide and a solution of sodium hydroxide, sodium metasilicate is formed by reaction 1:

$$mSiO_{2} + 2nNaOH + (p-n)H_{2}O \rightarrow$$

$$\rightarrow (nNa_{2}O \bullet SiO_{2} \bullet (p-x)H_{2}O) \bullet xH_{2}O +$$

$$+ (m-1)SiO_{2}$$
(1)

At temperatures below 130 °C, reactions of the formation of sodium silicate crystallohydrate and an aqueous layer from structurally oriented water occur. Part of the water is spent on the formation of sodium silicate crystallohydrates (fig 1, a) in the case of the presence in the composition of the required

nSiO₂-Si-O-Na-O
$$\overset{H}{H}$$
 nSiO₂-Si-O-Na-O $\overset{H}{H}_{H_{/}}^{H_{2}O}$
a b

Fig. 1. Diagram of the formation of structural bonds during hydration of the composition: a – sodium silicate crystallohydrates; b – water layer on the surface of crystal hydrates



Fig. 2. Diagram of the destruction of structural bonds during heating (1–2) and secondary chemisorption of water (3)



Fig. 3. Thermogravimetric curve of the charge composition based on microsilicon marshalite and sodium hydroxide solution

integer value of the number of moles of water. From a non-integer number of moles, an aqueous layer is formed on the surface of the crystallohydrates (fig 1, b) [1].

In the temperature range from $130 \,^{\circ}\text{C}$ to $310 \,^{\circ}\text{C}$, mass losses are observed associated with the removal of the water layer first (Fig. 2, 1) and then the dehydration of crystallohydrates with the transition to sodium silicate (Fig. 2, 2–3). In this case, partial chemisorption of moles of water occurs on the surface of dehydrated sodium silicate (Fig. 2, 3).

References

 Корнеев В. И., Данилов В. В. Жидкое и растворимое стекло. – СПб.: Стройиздат, 1996. – 216 с. With further heating, the secondary sorbed water is removed, up to the temperatures of the completion of the silicate formation process. When the temperature reaches the eutectic values, the charge melts with the formation of a melt. Residual silica dissolves in the resulting melt.

The developed model takes into account and complements the known data on chemical interaction. The developed model of physicochemical transformations fully corresponds to the results of thermogravimetric analysis (Fig. 3).

ESIPT-CAPABLE IMIDAZOLE DERIVATIVES WITH SINGLE AND DOUBLE PROTON TRANSFER: ABSORPTION AND EMISSION MECHANISMS

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Organic compounds with strong intramolecular hydrogen bonds of the O-H…Y and N-H…Y types (Y = O, NR) can demonstrate photoinduced intramolecular proton transfer reactions (Fig. 1, 2). The photoexcitation of such molecules in their most stable, or normal (N), form leads to the electron density redistribution followed by the excited state intramolecular proton transfer (ESIPT) reaction yielding the excited state tautomeric form (T). 1H-Imidazole derivatives establish one of iconic classes of ESIPT-capable compounds. This work represents a detailed photophysical characterization for L^{OH,OH}, which is the first example of ESIPT-capable imidazole derivatives wherein the imidazole moiety simultaneously acts as a proton acceptor and a proton donor, and for its monohydroxy congener



Fig. 1. Structural formulae of $L^{OH,OH}$ and $L^{H,OH}$

 $L^{H,OH}$ (Fig. 1). A slight structural difference between these two compounds leads to significant changes in their photoluminescence response. The number of OH…N proton transfer sites in these compounds (one for $L^{H,OH}$ and two for $L^{OH,OH}$) strongly affects the luminescence mechanism and color of emission: $L^{H,OH}$ emits in the light green region, whereas $L^{OH,OH}$ luminesces in the orange region (Fig. 3). According to joint experimental and theoretical studies, the main emission pathway of both compounds is associated with $T_1 \rightarrow S_0$ phosphorescence and not related to ESIPT. At the same time, $L^{OH,OH}$ also exhibits



Fig. 2. A typical photocycle of an ESIPT-fluorophore