## Processes of aerogels production with luminophores under supercritical conditions and their intensification

## Abstract

**Relevance of the research.** According to the decree of the Russian Federation Government on the approval of the state program "Scientific and technological development of the Russian Federation", the development of technologies for obtaining new hybrid and functional nanomaterials are priority areas of development of the global scientific, technological and innovative sphere. Such materials include aerogels with luminophores.

Luminophores are compounds capable of absorbing energy and converting it into light radiation. Due to this, these compounds are used in the production of energy-saving light sources, OLED display panels, biosensors and markers for the diagnosis of various diseases. But the main problem of using phosphors is their degradation in the air environment during long-term storage, use and transportation. One of the ways to preserve the quality and purity of phosphors is to place them in highly porous carrier matrices. In this work, it is proposed to use aerogels as carrier matrices, since they have a developed inner surface and a low density comparable to the density of air. The creation of new materials with luminophores based on aerogels with functional optical properties will significantly expand the traditional list of hybrid materials. In this case, inorganic aerogels with phosphors can be used in optoelectronics, photonics and optical instrumentation as a separate design element. In addition, biocompatible and non-toxic medical materials for humans can be produced on the basis of organic aerogels with phosphors.

The processes of obtaining aerogels with phosphors are complex and multi-stage, taking considerable time. Among all the stages of obtaining this material, the processes of gelation, solvent exchange and supercritical drying can be distinguished. Their fundamental research will make it possible to deepen the understanding of mass transfer processes, to propose new, more effective ways of conducting them, to intensify and optimize them.

In this work experimental researches of the processes of obtaining inorganic and organic aerogels with phosphors have been carried out. In addition, some processes of obtaining these materials were intensified. For this purpose, researches of combined processes of gelation, solvent exchange and supercritical drying in one apparatus under pressure were carried out. Experimental and theoretical researches of the phase state and

kinetics of phase transitions of two-component and three-component systems formed during the production of aerogels with luminophores have been carried out.

The work was carried out within the framework of agreement №075-15-2020-792 (unique identifier: RF-190220X0031) as part of the state assignment to the university on the topic "Nanobiotechnology in the diagnosis and therapy of socially significant diseases".

**The purpose of the work** – processes investigation and intensification of producing aerogels with luminophores under supercritical conditions.

## Tasks:

1. Experimental research of aerogels production with luminophores. Development of the injection and synthesis of luminophores in the aerogel matrix volume using supercritical technologies. Investigation of composition effect of initial components and process parameters on the structure of aerogels with luminophores and their luminescent characteristics.

2. Experimental and theoretical research of phase transitions kinetics two–component system "isopropanol - carbon dioxide" under various conditions. Determination of dependence of kinetic parameters on the system external parameters.

3. Mathematical modeling of multicomponent systems phase equilibrium, which formed during aerogels production with luminophores.

4. Experimental research of aerogels production with luminophores in the medium of supercritical carbon dioxide: processes of gelation and solvent exchange.

5. Intensification of gelation, solvent exchange and supercritical drying processes by conducting them in one apparatus under pressure.

**Scientific novelty.** For the first time a luminophores was synthesized in the aerogel matrix volume using supercritical technologies. When conducting a set of experiments for aerogels production with luminophores of various nature, the factors affecting the physicochemical, structural and luminescent properties were evaluated.

The kinetics of two- and three-component systems phase transitions in under pressure has been experimentally investigated. The influence of a highly porous gel on the speed of mass transfer processes has been researched.

Experimental research of the gelation and solvent exchange processes in pressurized gels have been carried out. The influence of the system phase equilibrium on solvent exchange under pressure process during the aerogels production has been researched.

The possibility of intensifying the producing aerogels with luminophores due to the stages of gelation, solvent exchange and supercritical drying in one apparatus is investigated.

**Theoretical and practical significance.** Producing aerogels processes of various natures with luminophores have been developed in three ways: the injection of luminophores at the solvent exchange stage, the synthesis of luminophores at the supercritical drying stage and with the use of supercritical adsorption. The luminophore material obtained by the first method (RF Patent  $N_{2}$  2757593) can be used in the production of light-emitting devices.

Organic aerogels with luminophores have been produced, which can be used as medical devices for the diagnosis and therapy of socially significant diseases.

The influence of the process parameters on the mass transfer coefficients has been established. The obtained data make it possible to reduce the time and resources required for mass transfer processes occurring in the aerogels production of various nature.

The main provisions for the defense. The experimental research results of the aerogels production of various nature in three ways: the injection of luminophores, the synthesis of luminophores at the stage of supercritical drying and with the use of supercritical adsorption; the effect of the production parameters on the final characteristics of materials.

Experimental curves of phase transitions kinetics of multicomponent systems that are formed during aerogels production under pressure; results of kinetic curves theoretical research.

Results of phase equilibrium mathematical modeling in multicomponent systems that are formed during aerogels production and luminophore materials based on them.

Results of processes experimental research of gelation and solvent exchange under pressure; combined of gelation, solvent exchange and supercritical drying processes in one apparatus.