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Investigation of the radiation-catalytic properties of nano-ZrO2 + nano-SiO2 systems in the process of producing hydrogen from water by IR spectroscopy

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This paper presents the results of Fourier-IR spectroscopic studies of the radiation decomposition of water in a heterogeneous system of nano-ZrO2 + nano-SiO2 + H2O at room temperature (T = 300 K) and exposure to γ-quanta in order to establish the role of intermediate-active particles (ion-radical groups) in these processes. The ratio of nano-ZrO2 and nano-SiO2 nanopowders varied as follows: 50% nano-ZrO2 + 50% nano-SiO2, 16.7% nano-ZrO2 + 83.3% nano-SiO2, and 83.3% nano-ZrO2 + 16.7% nano SiO2.

The Fourier IR absorption spectra were recorded on a Varian 640IR FT-IR spectrometer in the frequency range ν = 4000–400 cm –1 at room temperature. An analysis of the decomposition spectra of water in the γ-irradiated system of 50% nano-ZrO2 + 50% nano-SiO2 shows that new absorption bands (AB) are observed in the spectra at frequencies of 1570, 3142, and 3968 cm-1. Perhaps the bands at 1570 and 3142 cm -1 relate to adsorbed [O2] molecules in an uncharged form. The nanostructure of ZrO2 and SiO2 powders allows one to detect, along with the main absorption band (ν1 = 1570 cm-1), surface-adsorbed molecular oxygen and its AB in the overtone region (ν = 2ν1 = 3142 cm-1). The absorption band at ν = 3968 cm –1 refers to surface adsorbed molecular hydrogen [H2]. A change in the weight content of ZrO2 and SiO2 nanopowders results in a redistribution of AB intensities, which is due to a change in the surface states of the powders and their defects.

In the spectra, in the region of lattice vibrations of nano-SiO2 (ν = 1400–400 cm –1), AB with maxima of 472, 798, and 1095 cm –1 are detected. The observed bands are related to symmetric and asymmetric stretching vibrations of Si-O and Si-O2 –Si. A change in the weight ratios of ZrO2 and SiO2 nanopowders is accompanied by a redistribution of the intensities of the AB vibrations of Zr-O and Si-O.

In an unirradiated heterosystem, after water adsorption on the surface of zirconia and silicon dioxide in the region of stretching vibrations of hydroxyl (OH) groups, AB appear, which indicate the occurrence of molecular and dissociative forms of adsorption: the molecular form of adsorption (intense broad bands with maxima of 3240 and 3280 cm - 1 in the region of 3500–3000 cm-1) and dissociative chemisorption (relatively narrow bands with maxima of 3450, 3475, 3520, 3580 cm-1). The occurrence of two types of adsorption is also confirmed by the formation of AB in the region of deformation vibrations of OH with maxima at 1610, 1630, 1640, and 1680 cm –1.

Irradiation of a 50% nano-ZrO2 + 50% nano-SiO2 + H2O heterosystem with γ-quanta at room temperature (T = 300 K) leads to radiation decomposition of water and the formation of intermediate-active decomposition products. Among these products, the most interesting are the surface hydrides of zirconium and silicon. Thus, in the spectrum in the frequency range 2000–1700 cm –1, AB appear with maxima of 2100, 2000, 1995, and 1880 cm –1. These absorption bands belong to the stretching vibrations of Zr-H (1995, 1880 cm-1) and Si-H (2100, 2000 cm-1) and indicate the formation of surface zirconium and silicon hydrides of Zr-H, Zr-H2, Si-H, Si-H2 [6], among which the most stable forms are Zr-H2 and Si-H2. Unfortunately, we were not able to register AB oxygen containing intermediate-active surface particles of water decomposition. Since, these PPs overlap with the absorption bands of Si –O stretching vibrations (ν = 1200–900 cm –1).

In the Fourier IR absorption spectra of nano-ZrO2 + nano-SiO2 + H2O samples with adsorbed water, in the region of stretching vibrations of OH groups and water (ν = 4000–3000 cm-1), bands of hydrogen-bonded groups with maxima of 3580 are observed , 3520, 3475, 3450 cm-1, as well as adsorbed water molecules at 3280 and 3240 cm-1.

The radiation decomposition of water at room temperature is accompanied by a decrease in the intensity of the molecular water band, the formation of a number of AB hydrogen-bonded hydroxyl groups at 3350, 3500 cm-1, as well as new absorption bands at 3630 and 3690 cm-1. The last bands refer to isolated OH groups.

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