

FOURIER IR SPECTROSCOPY STUDY OF THE RADIATION-THERMAL DECOMPOSITION OF WATER IN THE nano-ZrO₂+nano-Al₂O₃+H₂O SYSTEM

T. N. Agayev, S. Z. Melikova[✉], N. N. Gadzhieva
*Institute of Radiation Problems NAS of Azerbaijan,
9, B. Vahabzadeh St., Baku, AZ-1143, Azerbaijan,
e-mail: sevincmelikova9513@gmail.com*

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This paper presents the results of Fourier transform infrared spectroscopic studies of the radiation-thermal decomposition of water in the heterogeneous system nano-ZrO₂+nano-Al₂O₃+H₂O at various weight ratios of nano-oxides in the temperature range $T = 373 \div 673$ K and during radiation exposure. It has been established that the main intermediate products of radiation-heterogeneous decomposition of water are molecular oxygen and other oxygen-containing radical ion groups generated by gamma irradiation, as well as surface hydrides of zirconium and aluminum. Based on a comparative analysis of changes in the intensity of the absorption bands of molecular water and surface hydroxyl groups characterizing nano-ZrO₂ and nano-Al₂O₃ as a function of temperature, the radiation-catalytic activity of nano-ZrO₂ was detected at a fixed value of the absorbed dose. $W_{RT}(H_2)$ and its radiation-chemical yields $G(H_2)$ were determined. A stimulating role in the radiation-thermal decomposition of H₂O in a heterogeneous nano-ZrO₂+nano-Al₂O₃ system ($T = 373 \div 673$ K) has been established.

Key words: Fourier IR spectroscopy, nano-zirconium oxide, nano-aluminum oxide, γ -irradiation, radiation-thermal decomposition.

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I. INTRODUCTION

Nanosized aluminum and zirconium oxide compounds are widely used as active components and an effective carrier of catalysts in various processes, including radiation-catalytic processes of hydrogen production from water [1–6]. Zirconium and aluminum oxides are also technologically important materials in the field of manufacturing ceramics, solid electrolytes, radiation detectors and materials for space and nuclear technologies. As it is known, reducing a particle size to nanoscale leads to a significant change in physical properties [3–4]. The dimensions of individual nanooxide particles are comparable to the mean free path of electrons, holes, and excited states produced by the action of ionizing radiation, which participate in the effective transformation and transfer of energy. To modify the physical and chemical properties, materials based on mixtures of nanoscale oxides are produced [7–9].

As a result of the interaction between the components, the concentration of surface acceptor centers changes, as well as the mechanical and physical properties of the components of the system. Information on the effect of the second component on the surface physical and chemical and radiation-catalytic properties of the binary system of nano-ZrO₂+nano-Al₂O₃+H₂O is limited. In the literature there is virtually no spectroscopic data on the radiation decomposition of water in a nano-ZrO₂+nano-Al₂O₃+H₂O system.

This paper presents the results of Fourier IR spectroscopic studies of the radiation-thermal decomposition of water in a heterogeneous system of nano-ZrO₂+nano-Al₂O₃+H₂O, in the temperature range $T = 373 \div 673$ K under the influence of γ -quanta, in order to establish the role of intermediate-active parti-

cles and to reveal the regularities of adsorption-active hydroxyl groups in these processes.

II. EXPERIMENTAL PART

ZrO₂ (particle size $d = 20–30$ nm) and Al₂O₃ (particle size $d = 20–60$ nm) nanopowders with a purity of 99.9% (Sky Spring Nanomaterials, USA) were used. The X-ray phase method established that the ZrO₂ sample has a monoclinic centrally symmetric crystal structure [10]. By the X-ray phase method, it was established that the nano-ZrO₂ sample has a monoclinic centrally symmetric crystal structure, and the nano-Al₂O₃ has -modification of the cubic structure. The values of specific surfaces are $S_{sp}(\text{nano-ZrO}_2) = 350 \text{ m}^2/\text{g}$ and $S_{sp}(\text{nano-Al}_2\text{O}_3) = 280 \text{ m}^2/\text{g}$. Before adsorption, samples of zirconium and aluminum dioxides were treated by thermovacuum at $T = 673$ K and pressure $P = 10^{-3}$ Pa for 8 h for cleaning from organic impurities and dehydroxylation of surfaces. The control over the surface cleanliness was carried out according to the intensity of IR bands caused by water and hydrocarbon contamination.

Fourier IR absorption spectra were recorded on a Varian 640 FTIR spectrometer in the frequency range $\nu = 4000 - 400 \text{ cm}^{-1}$ at room temperature. To remove the absorption spectra from a mixture of ZrO₂+Al₂O₃ nanopowders, pellets with a thickness of $50 \div 100 \mu\text{m}$ were pressed. The IR spectra of the samples were measured in special quartz cells with windows made of CaF₂, which made it possible to obtain spectra of adsorbed water, decomposed under the action of γ -irradiation by the method of [10]. The ratio of nanooxide components varied as 3:1, 1:1 and 1:3. When overlapping the bands related to different forms of adsorbed water and hydroxyl



groups, the total contour is decomposed into individual components according to the procedure [5]. This technique includes a program that takes into account the specificity of adsorbed molecules at the interface of the adsorbent-adsorbate. The intensities of the bands of adsorbed water molecules and hydroxyl groups in the systems under study were calculated. The values of the intensities given are the arithmetic average values obtained in four parallel independent experiments.

The adsorbate was bidistilled water, from which foreign gases were removed by repeated freezing in a trap with liquid nitrogen followed by pumping out. Adsorption of water vapor was studied by the method of [10]. The radiative decomposition of water in the system of nano-ZrO₂+nano-Al₂O₃+H₂O was carried out at room temperature ($T = 300$ K). Samples were irradiated on an isotope ⁶⁰Co source with a dose rate $dD_\gamma/dt = 0.14$ Gy/s. The dosimetry of the source was carried out by ferrosulfate and methane dosimeters [11]. The

absorbed dose of irradiation in the systems under investigation was determined by comparing the electron densities and was $D_\gamma = 30$ kGy.

III. RESULTS AND THEIR DISCUSSION

The IR spectrum of a mixture of nano-ZrO₂+nano-Al₂O₃ at a 1:1 ratio is shown in Fig. 1 (curve 1) and for nano-ZrO₂+nano-Al₂O₃+H₂O system — in Fig. 1 (curve 2). Then γ -irradiation of nano-ZrO₂+nano-Al₂O₃+H₂O systems was performed at same doses (curve 3), (curve 4) and $D_\gamma = 30$ kGy (curve 5). As can be seen from Fig. 1 (curve 1), the surface of a nano-ZrO₂+nano-Al₂O₃ mixture, which has undergone thermovacuum treatment, is pure, since there are no absorption bands due to the presence of water and hydrocarbon contaminants.

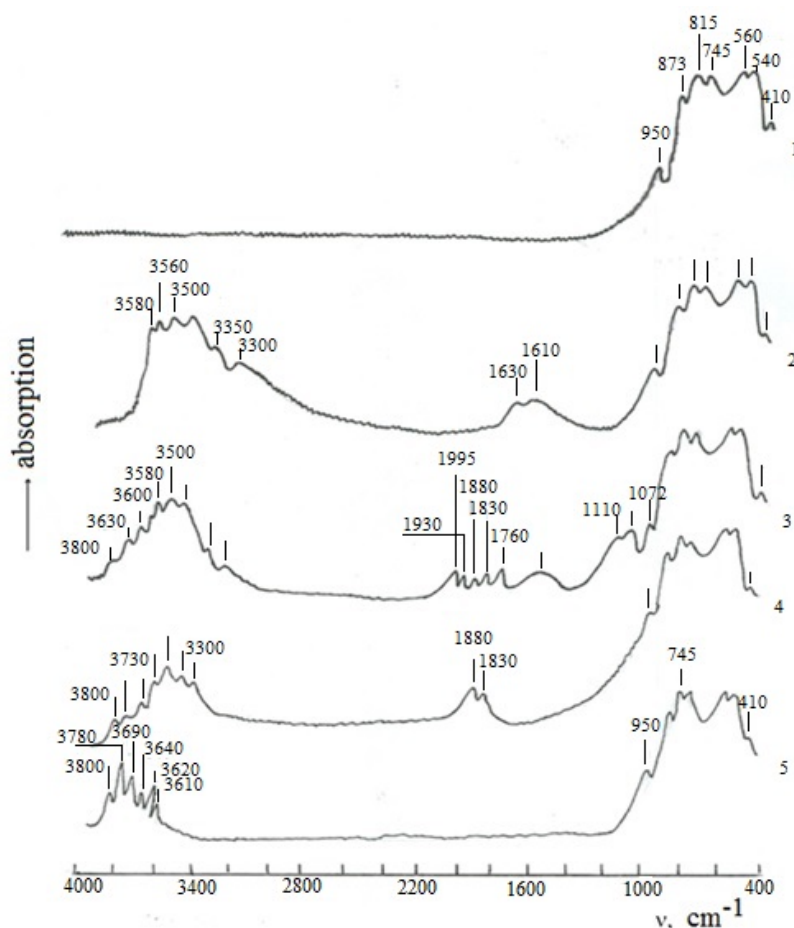


Fig. 1. Fourier IR spectra of nano-ZrO₂+nano-Al₂O₃, mixture, processed at 673 K (1), up to (2) and after the action of γ -irradiation on the system of nano-ZrO₂+nano-Al₂O₃+H₂O at 373 (3), 473 (4) and 673 K (5). The spectra were obtained with a weight ratio of nanooxide components (1:1) at a fixed dose of $D_\gamma = 30$ kGy.

Absorption bands with maxima at 950, 873, 815, 745, 560, 540, and 410 cm^{-1} were observed in the spectra, in the region of lattice vibrations of nano-ZrO₂ and nano-Al₂O₃. The 745 cm^{-1} band is referred to the asymmetric

vibration (Zr-O₂-Zr) [3,4]. The location and intensity ratio of absorption bands (AB) at 745–410 cm^{-1} indicate a monoclinic modification of the ZnO₂ nanopowder used [10]. The absorption bands refer to the stretching

vibration of Al–O, and the ABs at 873, 815, 560 and 540 cm^{-1} are apparently related to the presence of AlO_3 and AlO_6 -groups [1,3]. In studying adsorption processes and radiation-thermal decomposition of water, the lattice vibrations of zirconium and aluminum oxides and the constancy of their intensities are among the main criteria for the identification of the experimental conditions.

In the unirradiated heterosystem (nano- ZrO_2 +nano- Al_2O_3), after water adsorption ABs (Fig. 1, curve 1) with maxima 3580, 3560, appear in the region of stretching vibrations of hydroxyl (OH) groups 3500, 3450, 3350, 3300, 3280 and 3000 cm^{-1} , which indicates the flow of molecular and dissociative adsorption. The molecular form of adsorption corresponds to broad absorption bands at 3280 and 3300 cm^{-1} , while dissociative chemisorption corresponds to relatively narrow bands with maxima at 3580, 3560, 3500, 3450, 3350, and 3300 cm^{-1} (Fig. 1, curve 2). The presence of the two types of adsorption is confirmed by the formation of ABs in the region of OH deformation vibrations with centers of gravity at 1630 and 1610 cm^{-1} .

The irradiation of a heterosystem of nano- ZrO_2 +nano- Al_2O_3 + H_2O by γ -quanta (an absorption dose of $D_\gamma = 30\text{ kGy}$ at the temperature of $T = 373\text{ K}$) is accompanied by the appearance of new ABs in the $800\text{--}1000\text{ cm}^{-1}$ region with maxima at 1072, 1085, 1110 cm^{-1} , are associated with adsorption of molecular oxygen – the product of water decomposition on the surface of nano-oxides ZrO_2 and Al_2O_3 , indicating the formation of ion radicals of oxygen in the π -form, i. e. O^{2-} .

Thus, Fourier IR spectroscopy allows recording the intermediate products of the radiation-thermal decomposition of water in the system of nano- ZrO_2 +nano- Al_2O_3 + H_2O on the oxide surface. Among these products, surface zirconium and aluminum hydrides are most intense. Thus, starting from the temperature of $T = 373\text{ K}$ in the spectrum, in the frequency range $2000\text{--}1700\text{ cm}^{-1}$ there appear ABs appear with maxima at 1760, 1830, 1880, 1920 and 1995 cm^{-1} , whose intensities are redistributed with the growth of temperature. These ABs refer to the stretching vibrations of Zr–H and Al–H, indicating the formation of surface hydrides of the Zr–H, ZrH_2 , Al–H, AlH_2 and AlH_3 types. Among these hydrides, the most stable forms are ZrH_2 ($\nu = 880\text{ cm}^{-1}$) and AlH_3 ($\nu = 1830\text{ cm}^{-1}$) [12–14].

Changes in the valence vibrations of hydroxyl (OH) groups associated with the radiation-thermal decomposition of water in a heterogeneous system of nano- ZrO_2 +nano- Al_2O_3 + H_2O are shown in Fig. 1 (curves 3–5). In the Fourier IR absorption spectra of samples of a nano- ZrO_2 +nano- Al_2O_3 mixture with adsorbed water, in the region of stretching vibrations of OH groups and water ($\nu = 4000\text{--}3000\text{ cm}^{-1}$), the ABs of hydrogen bonded groups with maxima at 3580, 3500 and 3450 cm^{-1} , as well as adsorbed water molecules at 3280 cm^{-1} are observed (Fig. 1, curve 3).

The radiation-thermal decomposition of water at $T = 373\text{ K}$ is accompanied by a decrease in the intensities of the ABs of molecular water and hydrogen-bonded

hydroxyl groups, as well as the formation of new bands of isolated OH groups at 3630 and 3690 cm^{-1} .

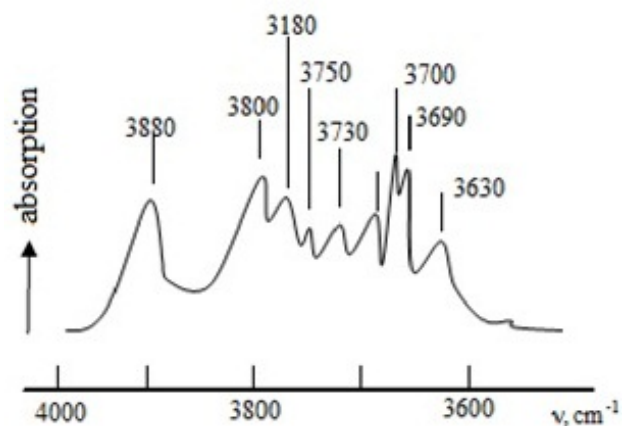


Fig. 2. Absorption bands region of the isolated OH groups in the nano- ZrO_2 +nano- Al_2O_3 system to the Zr and Al oxides.

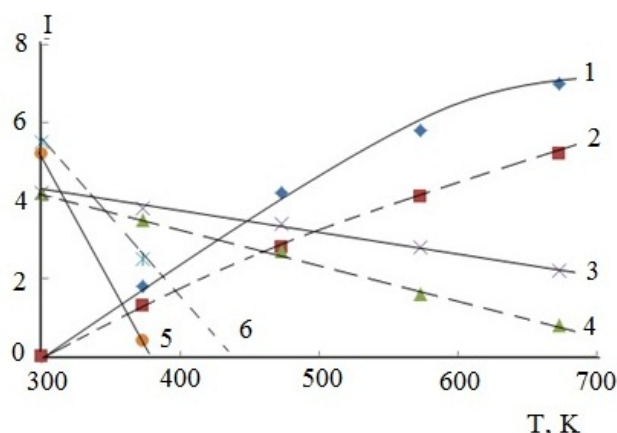


Fig. 3. Dependences of the intensities of bands of isolated (1, 2) and hydrogen-bonded (3, 4) surface OH groups, as well as adsorbed water molecules (5, 6) on the temperature of radiation-thermal processes of water decomposition in the heterogeneous system of nano- ZrO_2 +nano- Al_2O_3 + H_2O (the dependences for nano- ZrO_2 are shown by solid lines, and for nano- Al_2O_3 -by dotted lines), ($D_\gamma = 30\text{ kGy}$).

An increase in temperature to 473 K is accompanied by a decrease in the intensity of H-bound and an increase in the intensity of bands of isolated OH groups at 3630 and 3690 cm^{-1} (Fig. 1, curve 4). The temperature rise up to 673 K leads to complete decay of molecular water and partial decay of H-bonded OH groups (curves 3–5). At $T = 473\text{ K}$, new AB appear in the IR spectrum at 3780 and 3800 cm^{-1} . According to the notions of the structure of hydroxyl nano oxides of zirconium and aluminum [2, 15–16], the observed new bands correspond to hydroxyl groups differing in coordination numbers. For example, according to the concept of the structure of the hydroxyl coating of nano zirconium oxide, the observed new ABs correspond to hydroxyl groups that differ in coordination number: terminal, i. e. isolated OH groups of type I, isolated on Zr cations (AB 3780 cm^{-1}), two coordinated bridging types II (AB 3750 cm^{-1}) and three coordinated

bridging types III (AB 3640 and 3690 cm^{-1}). According to [10], these ABs can be attributed to the hydroxyl groups of ZrO_2 , mainly in the surface areas with the (111) and (110) face structure of the fluorite-like modification. Note that in the IR spectra of ZrO_2 dispersed powders with micro-sized particles, only isolated OH groups of types I and II were detected. According to [12], in nano-aluminum oxide, depending on the coordination number, there are also isolated hydroxyl groups of 3 types: isolated OH-type group I (AB 3880, 3800 cm^{-1}), type II (AB 3770 cm^{-1}) and type III (AB 3730, 3700 cm^{-1}). To identify spectrokinetic patterns, i. e. changes in the intensities of ABs of molecular water and surface OH groups, depending on the processing temperature, the IR absorption spectra of their regions were obtained under special recording conditions. As an example, Fig. 2 shows the AB region of the OH groups that appear during the radiolysis of water in the nano- ZrO_2 +nano- Al_2O_3 system to the Zr and Al oxides. Nine absorption bands with good resolution are clearly visible, four of which (AB 3780, 3750, 3690 and 3640 cm^{-1}) are associated with ZrO_2 , and five (AB 3880, 3800, 3770, 3730 and 3700 cm^{-1}) with Al_2O_3 .

The analysis of the changes in the intensities of the ABs of molecular water, H-bound and isolated hydroxyl groups at a fixed dose of radiation ($D_\gamma = 30$ kGy),

depending on the temperature of the process of the radiation-thermal decomposition of water, shows that there are antipate dependencies between them. Thus, an increase in temperature from 473 to 673 K leads to the complete and partial decomposition of molecular water and H-bonded OH groups and the formation of isolated OH groups. This leads to a decrease in the intensity of H-bound and, vice versa, to an increase in the intensity of isolated OH groups.

Figure 3 shows the dependences of the AB intensities on the temperature for isolated (at 3690 and 3700 cm^{-1} (curves 1, 2)) and hydrogen-bonded (at 3450 and 3500 cm^{-1} (curves 3, 4)) surface OH-groups, as well as adsorbed water molecules (at 3280 and 3300 cm^{-1} (curves 5, 6)) during the radiation-thermal decomposition of water in the heterogeneous system of nano- ZrO_2 +nano- Al_2O_3 + H_2O . Solid lines show the dependence for nano- ZrO_2 , and the dashed lines — for nano- Al_2O_3 . Comparing these relationships, we see that an increase in temperature from 373 to 673 K leads to antipate dependences of H-bound and isolated surface hydroxyl groups. Changes in the ratio of the concentrations of ZrO_2 and Al_2O_3 nanopowders (1:3, 1:1 and 3:1) in the Fourier IR absorption spectra are accompanied by a redistribution of the intensities of the ABs of molecular water, H-bonded and isolated OH groups.

No.	System	T , K	$W_T(\text{H}_2)$, molecule/g·s	$W_{RT}(\text{H}_2)$ molecule/g·s	$G(\text{H}_2)$ molecule/100 eV
1	n- ZrO_2	373	$1.0 \cdot 10^{13}$	$5 \cdot 10^{13}$	4.5
2	n- Al_2O_3		$0.69 \cdot 10^{13}$	$2.78 \cdot 10^{13}$	2.75
3	n- ZrO_2 + n- Al_2O_3 (3:1)		$0.84 \cdot 10^{13}$	$4.2 \cdot 10^{13}$	4.0
4	n- ZrO_2 + n- Al_2O_3 (1:1)		$0.67 \cdot 10^{13}$	$3.34 \cdot 10^{13}$	3.1
5	n- ZrO_2 + n- Al_2O_3 (1:3)		$0.51 \cdot 10^{13}$	$2.91 \cdot 10^{13}$	2.7

Table 1. Values of formation rates $W(\text{H}_2)$ and of chemical yields of molecular hydrogen $G(\text{H}_2)$ at radiation-thermal (RT) and thermal (T) decomposition of water into nano- ZrO_2 , nano- Al_2O_3 and binary system of nano- ZrO_2 +nano- Al_2O_3 at temperature $T = 373$ K.

No.	System	T , K	$W_T(\text{H}_2)$, molecule/g·s	$W_{RT}(\text{H}_2)$ molecule/g·s	$G(\text{H}_2)$ molecule/100 eV
1	n- ZrO_2	473	$5.56 \cdot 10^{13}$	$2.08 \cdot 10^{14}$	8.35
2	n- Al_2O_3		$2.22 \cdot 10^{13}$	$5.83 \cdot 10^{13}$	4.15
3	n- ZrO_2 + n- Al_2O_3 (3:1)		$5.02 \cdot 10^{13}$	$1.81 \cdot 10^{14}$	7.5
4	n- ZrO_2 + n- Al_2O_3 (1:1)		$4.45 \cdot 10^{13}$	$1.0 \cdot 10^{14}$	6.7
5	n- ZrO_2 + n- Al_2O_3 (1:3)		$2.57 \cdot 10^{13}$	$6.78 \cdot 10^{13}$	4.8

Table 2. Values of formation rates $W(\text{H}_2)$ and of chemical yields of molecular hydrogen $G(\text{H}_2)$ at radiation-thermal (RT) and thermal (T) decomposition of water into nano- ZrO_2 , nano- Al_2O_3 and binary system of nano- ZrO_2 +nano- Al_2O_3 at temperature $T = 473$ K.

The decomposition of hydrogen-bonded hydroxyl groups is accompanied by the accumulation of isolated surface OH groups. Under radiation-thermal action, the water desorption process is correlated by the decay of H-bound and the accumulation of isolated surface OH groups for nano- ZrO_2 , which is much more effective than

nano- Al_2O_3 [17, 18]. This indicates the catalytic activity of nano- ZrO_2 in the process of the radiation-thermal decomposition of water in the heterogeneous system of nano- ZrO_2 +nano- Al_2O_3 + H_2O in the temperature interval $T = 373 \div 673$ K.

No.	System	T , K	$W_T(\text{H}_2)$, molecule/g·s	$W_{RT}(\text{H}_2)$ molecule/g·s	$G(\text{H}_2)$ molecule/100 eV
1	n-ZrO ₂	673	$2.78 \cdot 10^{14}$	$6.94 \cdot 10^{14}$	24.7
2	n-Al ₂ O ₃		$4.17 \cdot 10^{13}$	$9.44 \cdot 10^{13}$	8.6
3	n-ZrO ₂ + n-Al ₂ O ₃ (3:1)		$2.59 \cdot 10^{14}$	$4.45 \cdot 10^{14}$	21.2
4	n-ZrO ₂ + n-Al ₂ O ₃ (1:1)		$1.52 \cdot 10^{14}$	$2.61 \cdot 10^{14}$	12.9
5	n-ZrO ₂ + n-Al ₂ O ₃ (1:3)		$1.17 \cdot 10^{14}$	$1.93 \cdot 10^{14}$	8.1

Table 3. Values of formation rates $W(\text{H}_2)$ and of chemical yields of molecular hydrogen $G(\text{H}_2)$ at radiation-thermal (RT) and thermal (T) decomposition of water into nano-ZrO₂, nano-Al₂O₃ and binary system of nano-ZrO₂+nano-Al₂O₃ at temperature $T = 673$ K.

Tables 1–3 show the experimentally obtained values of the rate of formation of the final decomposition product of molecular hydrogen (H_2) for the thermal and radiation-thermal processes of the decomposition of $W_T(\text{H}_2)$ and $W_{RT}(\text{H}_2)$, as well as its yields $G(\text{H}_2)$ in depending on the ratio of ZrO₂ and Al₂O₃ nanopowders at different temperatures ($T = 373, 473$ and 673 K). As can be seen from the tables, the highest values of $G(\text{H}_2)$ in this system are observed at the concentration of 75 wt.% nano-ZrO₂ (3:1), which is due to the most active surface-active centers of the type Zr^{4+} . A comparative analysis of the values of $W(\text{H}_2)$ and $G(\text{H}_2)$ shows that in the temperature range $T = 373 \div 673$ K, the rates and yields of the formation of H_2 in the RT processes are significantly higher compared with the T process. This indicates the stimulating role of radiation in these processes [19].

IV. CONCLUSION

The radiation-thermal decomposition of water in the nano-ZrO₂+nano-Al₂O₃+H₂O heterosystem in the temperature range $373 \div 673$ K at the ratio of nano-oxides

(3:1, 1:1 and 1:3) was studied by Fourier IR spectroscopy and at a fixed value of the absorbed dose ($D_\gamma = 30$ kGy). It is shown that the adsorption of water in a mixture of nano-oxides of zirconium and aluminum occurs by molecular and dissociative mechanisms.

The intermediate products of the radiation-heterogeneous decomposition of water are ion-radicals of molecular oxygen, surface hydrides of zirconium and aluminum, as well as hydroxyl groups. Dependences of the intensities of absorption bands of molecular water and surface hydrogen-bonded and isolated hydroxyl groups characterizing nano-ZrO₂ and nano-Al₂O₃ on temperature have been studied. Based on a comparative analysis of these relationships, the radiation-catalytic activity of nano-ZrO₂ in the radiation-thermal process of water decomposition has been revealed.

The values of the rates of formation of $W(\text{H}_2)$ and the radiation-chemical yields of molecular hydrogen $G(\text{H}_2)$ during the radiation-thermal and thermal decomposition of water into nano-ZrO₂, nano-Al₂O₃ and the binary system of nano-ZrO₂+nano-Al₂O₃ were determined. The stimulating role of radiation during the radiolysis of H₂O in the temperature range $T = 373 \div 673$ K has been established.

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ФУР'Є-ІЧ-СПЕКТРОСКОПІЯ ВИВЧЕННЯ РАДІАЦІЙНО-ТЕРМАЛЬНОГО РОЗКЛАДАННЯ ВОДИ В СИСТЕМІ $\text{nano-ZrO}_2 + \text{nano-Al}_2\text{O}_3 + \text{H}_2\text{O}$

Т. Н. Агаєв, С. З. Мелікова, Н. Н. Гаджієва
*Інститут радіаційних проблем НАН Азербайджану,
вул. Б. Вагабаде, 9, Баку, AZ 1143, Азербайджан,
e-mail: sevinmelikova9513@gmail.com*

У цій роботі подано результати інфрачервоних спектроскопічних досліджень перетворення Фур'є радіаційно-термічного розкладання води в гетерогенній системі $\text{nano-ZrO}_2 + \text{nano-Al}_2\text{O}_3 + \text{H}_2\text{O}$ за різних вагових співвідношень наноксидів у діапазоні температур $T = 373 \div 673 \text{ K}$ і під час радіаційного опромінення. Установлено, що основними проміжними продуктами радіаційно-гетерогенного розкладання води є молекулярний кисень та інші кисневмісні радикальні йонні групи, що утворюються гамма-опроміненням, а також поверхневі гідриди цирконію та алюмінію. На основі порівняльного аналізу змін інтенсивності смуг поглинання молекулярної води та поверхневих гідроксильних груп, що характеризують nano-ZrO_2 та $\text{nano-Al}_2\text{O}_3$ як функцію температури, виявлено радіаційно-каталітичну активність nano-ZrO_2 за встановленого значення поглиненої дози. Визначено $W_{\text{RT}}(\text{H}_2)$ та його радіаційно-хімічні виходи $G(\text{H}_2)$. Установлено стимулювальну роль у радіаційно-термічному розкладанні H_2O в гетерогенній системі $\text{nano-ZrO}_2 + \text{nano-Al}_2\text{O}_3$ ($T = 373 \div 673 \text{ K}$).

Ключові слова: фур'є-ІЧ-спектроскопія, нано-цирконієвий оксид, нано-алюмінієвий оксид, γ -опромінення, радіаційно-термічне розкладання