



NANO-SI/H₂O SİSTEMİNDƏ SUYUN RADİASIYA-TERMİKİ PARÇALANMASININ FURYE İNFRAQIRMIZI SPEKTROSKOPİYA TƏDQIQI

Bəşirova Sevinc Məmmədhasən qızı- f.ü.f.d., Təbii Ehtiyatların Kosmik Tədqiqi İnstitutu,
bashirovasevinc1@gmail.com

Xülasə. İonlaşdırıcı şüaların nanohissəciklərə təsiri, materialların kimyəvi və fiziki xüsusiyyətlərini dəyişdirə bilər. Furiye infraqırmızı spektroskopiyası vasitəsilə bu proseslərin tədqiqi, nanomaterialların radiasiya mühitindəki davranışını daha yaxşı anlamağa və yeni tətbiq sahələrinin inkişafına yol açır. Bu tədqiqat, həm elmi, həm də praktiki baxımdan əhəmiyyət kəsb edir. Si/H₂O (50, 100, 300-500 nm) yaradılan sistemlərdə gedən termiki və ionlaşdırıcı şüaların (⁶⁰Co, P=18,17 rad/san, T=300K, 373, 473, 573, 623 və 673K) təsirlə radiasiya-termiki proseslər zamanı alınan məhsullar və aralıq məhsulları tədqiq etmək üçün Furiye infraqırmızı spektroskopiyasından istifadə edilmişdir. İonlaşdırıcı şüaların təsiri ilə nano-Si/H₂O heterosistemində otaq temperaturunda (T=300K) suyun parçalanması zamanı aralıq - aktiv məhsullar (hidridlər və hidroksil qruplar) əmələ gəlməsi müəyyən edilmişdir.

Açar sözlər: qamma şüalanma, nanohissəcik, radioliz, Furiye infraqırmızı spektrometri

STUDY OF RADIATION-THERMAL DECOMPOSITION OF WATER IN THE NANO-SI/H₂O SYSTEM USING FOURIER INFRARED SPECTROSCOPY

Bashirova Sevinj Mammadhasan- PhD in physics, Institute of Natural Resources,
bashirovasevinc1@gmail.com

Abstract. The effect of ionizing radiation on nanoparticles can change the chemical and physical properties of materials. The study of these processes by means of Fourier infrared spectroscopy leads to a better understanding of the behavior of nanomaterials in the radiation environment and the development of new fields of application. This research is important from both scientific and practical point of view. Radiation-thermal under the influence of thermal and ionizing rays (⁶⁰Co, P=18.17 rad/sec, T=300K, 373, 473, 573, 623 and 673K) in the systems created in Si/H₂O (50, 100, 300-500 nm) Fourier infrared spectroscopy was used to study the products and intermediates obtained during the processes. The formation of intermediate - active products (hydrides and hydroxyl groups) during water splitting at room temperature (T=300K) in the nano-Si/H₂O heterosystem under the influence of ionizing rays was determined.

Keywords: gamma radiation, nanoparticle, radiolysis, Fourier infrared spectrometer

Introduction. Fourier infrared spectroscopy of nanoparticles is a powerful tool for the study of materials at the micro- and nanoscale, with broad applications in modern science.

There are various methods exist for investigating the intermediate products and end products resulting from the radiation-induced heterogeneous processes during the decomposition of water in metal and metal oxide/water systems of different sizes (nano-, micro-, and porous). One of these methods is infrared spectroscopy [1], [2]. This paper presents the results obtained from the spectroscopic investigation of radiation-thermal decomposition of water in the nano-Si/H₂O system.

Methodology. Using the Fourier infrared spectroscopy method, intermediate products such as silicon hydrides and hydroxyl groups obtained from the radiation-thermal decomposition of water in

the nano-Si/H₂O systems were recorded in the temperature range of $T=300$ - 673 K. The effect of γ -quanta ($T=473$ K, $D=4$ kQr) on the nano-Si/H₂O system was examined, and changes in the absorption bands of water molecules and OH groups were observed.

In Figure 1, the infrared spectra of the surface-treated nano-Si (curve 1) and the adsorption of water on the nano-Si surface (curve 2) recorded at room temperature ($T=300$ K) are presented. From both curves (curve 1 and 2), it can be seen that the surface of the thermally treated nano-Si sample is clean, with no absorption bands corresponding to water and hydrocarbon compounds observed on its surface. Water molecules on the silicon surface exist in a dissociative and molecular adsorbed state, coordinated with an unsaturated coordination number (Si) and partly on positive Si⁺ centers. On the other hand, the spectra obtained after irradiating the systems created by the adsorption of water on the nano-Si surface with γ -quanta at doses of 25 kQr at temperatures of $T=300$ (3), 473 (4), and 673K (5) are shown in Figure 1.

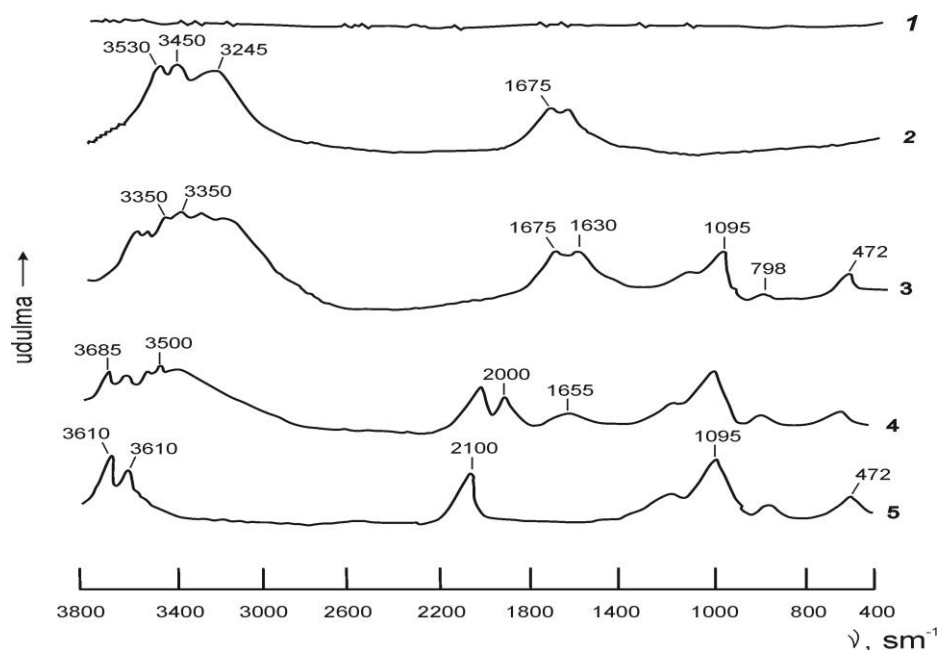


Figure 1. Fourier infrared spectra obtained from the surface-treated nano-Si (1), the system created by the adsorption of water on the nano-Si surface (2), and the systems created by the adsorption of water on the nano-Si surface after irradiation with γ -quanta at a dose of 25 kQr at temperatures of $T=300$ (3), 473 (4), and 673K (5)

Results and discussions. In the unirradiated heterosystem, after the adsorption of water, absorption bands (3500 - 3000 cm^{-1}) are observed on the surface of nano-Si, indicating the occurrence of molecular adsorption of OH groups in the region of vibrational modes (maximum broad intense band at 3245 cm^{-1}) and dissociative chemisorption (maximum narrow bands at 3450 and 3530 cm^{-1}) (curve 2). The occurrence of these two types of adsorption is confirmed by the presence of absorption bands with maxima at 1630 and 1675 cm^{-1} in the deformation mode region of the OH vibrations.

At room temperature ($T=300$ K), under the influence of γ - quantum, water splitting products and active intermediates are formed in nano-Si/H₂O heterosystems (curve 3). Among these products, surface hydrides of silicon are of particular interest. In the spectrum, the maximum absorption bands at 2100 and 2000 cm^{-1} in the frequency range of 2000 - 1700 cm^{-1} indicate the presence of Si – H valence oscillations, as well as the formation of Si – H and Si – H₂ type silicon hydrides. Among them, Si – H₂ has a more stable form. It was not possible to record the absorption bands of intermediate active products containing oxygen, because those bands and the absorption bands of valence oscillations of Si – O ($\nu=1200$ – 900 cm^{-1}) cover each other. During water splitting, maximum absorption bands of 472 , 798 , 1025 cm^{-1} (curve 3) are observed in the region of $\nu=1400$ - 400 cm^{-1} , which belong to Si – O and Si – O – Si symmetric and asymmetric valence oscillations. This also

indicates the oxidation of the nano-Si surface, as the intensity of these bands increases with the increase of the decomposition temperature (curve 4, 5).

Absorption of hydroxyl groups during thermal and radiation-thermal decomposition of water under the influence of γ - quanta ($P=18.17$ rad/sec) and temperature ($T=300, 373, 473, 573, 623$ and 673 K) in the Nano-Si/ H_2O system Kinetic dependences of relative optical densities (D/D_0) of the bands on contact time were studied. Figure 2 shows the dependences of the thermal (dotted) decomposition of water at $T=473$ K.

With the increase of the contact time, there is an increase of hydrogen-bonded OH – groups ($\nu=3685$ cm^{-1}). Comparative analysis shows that the rate of decomposition of H-bonded groups (curve 1) and collection of isolated OH-groups (curve 2) in the radiation-thermal process is greater than the rate of decomposition in the thermal process (curve 1', 2'). This shows the stimulating role of radiation and agrees with the values of molecular hydrogen generation rate and energy output [3].

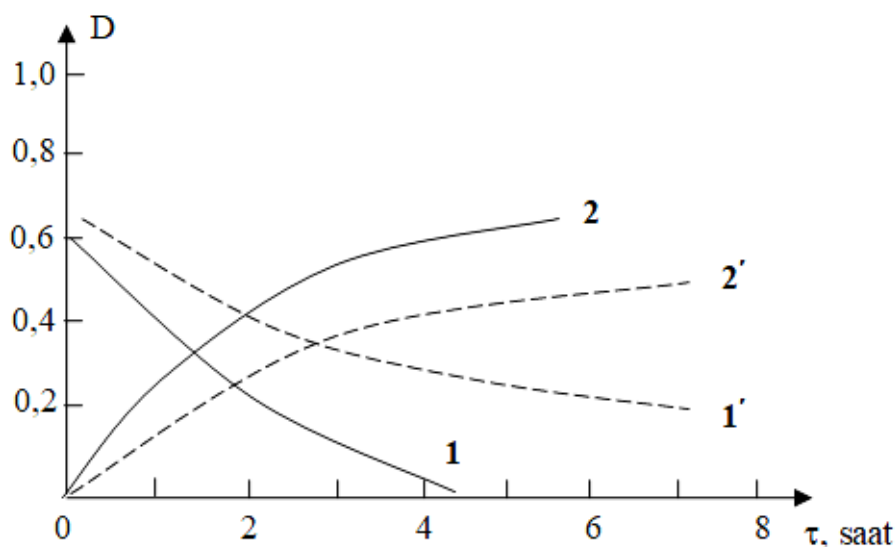


Figure 2. H-bond (1, 1') during radiation-thermal (1,2) and thermal (1', 2') splitting of water in Nano-Si/ H_2O system ($T=473$ K) and time dependence of relative optical densities of absorption bands of isolated OH groups (2', 2')

Conclusion. When studying the radiation-thermal decomposition of water in the Nano-Si/ H_2O system by Fourier Infrared spectroscopy, we can summarize the following ideas:

1. It was determined that the rate of decomposition of H-bonded groups and the collection of isolated OH-groups during the radiation-thermal decomposition of water in the nano-Si/ H_2O system is greater than the rate of decomposition in the thermal process. This also shows the stimulating role of radiation and agrees with the values of molecular hydrogen generation rate and energy output.

2. It was determined that intermediate active products (hydrides and hydroxyl groups) are formed during water splitting at room temperature ($T=300$ K) in the nano-Si/ H_2O heterosystem under the influence of γ -quanta.

References

1. Agayev, T. N., Gadzhieva, N. N., Melikova, S. Z., İmanova, G. T., & Faradjade, I. A. (2018). An IR spectroscopic study of the gamma radiation on the nano- ZrO_2 + nano- SiO_2 + H_2O systems. *Protection of Metals and Physical Chemistry of Surface*, 54(5), 813-816.
2. Agayev, T. N., Gadzhieva, N. N., & Melikova, S. Z. (2018). Fourier transform IR spectroscopic study of nano- ZrO_2 + nano- SiO_2 + H_2O systems upon the action of gamma radiation. *Journal of Applied Spectroscopy*, 85(2), 365-369.

3. Агаев, Т. Н., Гаджиева, Н. Н., & Меликова, С. З. (2017). Радиационное разложение воды в системе $n\text{-ZrO}_2 + n\text{-SiO}_2 + \text{H}_2\text{O}$. In Международный форум «Ядерная наука и технологии», посвященный 60-летию Института Ядерной физики (pp. 96-98).
4. Bashirova, S. M., Jafarov, Y. D., & Aliyev, S. M. (2017). Dependence of the yield of molecular hydrogen obtained from radiation-heterogeneous decomposition of water on particle size of silica and filling rate of particle surface of water in $\text{Si} + \text{H}_2\text{O}$ system by the influence of gamma-quanta. Azerbaijan National Academy of Sciences Institute of Radiation Problems, Journal of Radiation Researches, 4(2), 16-23.
5. Джафаров, Я. Д., Баширова, С. М., Гарибов, А. А., & Эюбов, К. Т. (2019). Получение молекулярного водорода, образованного термическим и радиационно-термическим превращением воды в системе $\text{nano-Si} + \text{H}_2\text{O}$. Вопросы атомной науки и техники (ВАНТ), Национальный научный центр "Харьковский физико-технический институт", 1, 55-60.
6. Баширова, С. М. (2019). Влияние массы кремния на процесс радиолитического разложения воды при воздействии γ -квантов на суспензионную систему $\text{nano-Si/H}_2\text{O}$. In EurasiaScience XXV Международная научно-практическая конференция (pp. 3-4). Научно-издательский центр "Актуальность.РФ".
7. Bashirova, S. (2024). Fourier Infrared Spectroscopy study of radiation-thermal water decomposition in $\text{Nano-Si/H}_2\text{O}$ system. In 21st international conference on defects in insulating materials – ICDIM 2024, L.N. Gumilyov Eurasian National University, 19-23 August 2024.
8. Jafarov, Y. D., Bashirova, S. M., Mardanov, I. J., & Imanova, G. T. (2023). Obtaining molecular hydrogen from water radiolysis in the nano-SiO_2 ($d = 20 \text{ nm}$) / H_2O system under the influence of γ -quanta. Cambridge University Press, Experimental Results UK, 1-11.
9. Qəribov, A. A., Ağayev, T. N., Bəşirova, S. M., İmanov, G. T., Əliyev, A. Q., & Cəfərov, Y. D. (2024). Mechanism of hydrogen production in the processes of radiation-heterogeneous splitting of water with the presence of nano-metal and Nano-MeO_1 . East European Journal of Physics, 460-475.
10. Cəfərov, Y. D., Bəşirova, S. M., İmanova, G. T., & Əliyev, S.M. (2023). Study of molecular hydrogen in the $\text{nano-SiO}_2 / \text{H}_2\text{O}$ system under the influence of γ -quanta. In X International Scientific Conference "Actual Problems of Solid State Physics" (APSSP-2023), Belarus, 22-26 May 2023 (p. 358).
11. Bashirova, S. M. (2022). The impact of silicon mass on the radiolysis process occurring under the influence of gamma-quanta on $\text{nano-Si} / \text{H}_2\text{O}$ suspension system. In IV International Scientific Forum "NUCLEAR SCIENCE AND TECHNOLOGIES" dedicated to the 65th anniversary of the Institute of Nuclear Physics (pp. 106). Institute of Nuclear Physics Ministry of Energy of the Republic of Kazakhstan.
12. Bəşirova, S. M., & Cəfərov, Y. D. (2016). $\text{Si} + \text{H}_2\text{O}$ sistemində suyun radiolizi prosesində kütlə effekti. Azərbaycan Milli Aerokosmik Agentliyinin xəbərləri, 2(19), 52-60.
13. Theophanides, T. (2012). Infrared Spectroscopy- Materials Science, Engineering and Technology, Introduction to Infrared Spectroscopy. National Technical University of Athens

Məqaləyə istinad: Bəşirova, S.M. (2025). Nano-Si/H₂O sistemində suyun radiasiya-termiki parçalanmasının Furye infraqırmızı spektroskopiyaya tədqiqi. Elmi Əsərlər/Scientific Works, AzMIU, 1, 113-116

For citation: Bashirova, S.M. (2025). Study of radiation-thermal decomposition of water in the Nano-Si/H₂O system using Fourier infrared spectroscopy. Elmi Əsərlər/Scientific Works, AzUAC, 1, 113-116

Redaksiyaya daxil olma/Received 11.09.2024

Çapa qəbul olunma/Accepted for publication 11.11.2024