Importance of the radiations in water splitting for hydrogen generation

Gunel Imanova^{1*}, Ilkhom Bekpulatov², Anar Aliyev¹ and Sami Barkaoui³

¹Institute of Radiation Problems, Ministry of Science and Education Republic of Azerbaijan, Baku AZ-1143, Azerbaijan

²Tashkent State Technical University, Tashkent, Uzbekistan

³Materials Processing and Analysis Laboratory INRAP, Technopôle, Sidi Thabet 2020, Tunisia

Abstract

The review article examines the production of molecular hydrogen from the decomposition of water by various irradiation methods. The article shows different types of radiation: UV radiation, visible radiation, gamma radiation, X-ray radiation and neutron radiation. Electrons generated by radiation inside a nanoparticle of radius R suspense in fluid water are diffused with equal probability in all directions inside the particle and gradually lose their kinetic energy as a result of elastic and inelastic collisions. Some of these electrons are transported to the nanoparticle surface during the physical and physicochemical stages of the process and emitted into the water. It is extremely important for the formation of nanostructured materials after exposure to ordered nanostructure from the new phase with a period of a few nanometers, promoting the preservation of the properties of materials under high irradiation.

Introduction

To ensure safety, it is important to be sure of the tightness of the system during the use of hydrogen in terms of preventing accidents and studying these processes by developing methods of accident management can diminish the adverse effects. The literature review shows that the theoretical and experimental results of these processes are an excellent basis for process management, safe operation of reactors and safety of hydrogen energy.

This should be taken into account in the study and analysis of oxidation processes under the influence of irradiation. All the considerations about the effect of radiolysis on oxidation processes are justified by the effect on the kinetics of oxidation processes in the aquatic environment [1,2].

Thus, in water and nuclear reactors, in the fields of radiation materials science, the composition of construction materials, storage containers and the lifespan of nuclear waste is in contact with solid surfaces of waste materials and the study of hydrogen explosives in H_2O_2 leads to problem-solving as a result [3,4].

Based on these results, the increase in the formation of molecular hydrogen occurs in the presence of oxide and

More Information

*Address for correspondence: Gunel Imanova, Institute of Radiation Problems, Ministry of Science and Education Republic of Azerbaijan, Baku AZ-1143, Azerbaijan, Email: radiasiya555@rambler.ru

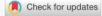
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water systems. Oxygen production requires less energy than hydrogen. The radiolysis process of GeO_2 generates helium ion radicals at 5 MeV, which is lower than ZrO_2 in the formation of molecular hydrogen as a result of γ -rays [5].

The resulting radicals weaken their oxidation and cause their destruction. Otherwise, the total potential of hydroxyl radicals (OH⁻) has very strong oxidizing properties and is equal to E^o (HO⁺/ H₂O) = + 2.7 eV. Various radicals are formed as a result of radiolysis processes. However, these reactions are time-depended and have been obtained experimentally. The mechanism explaining the received results is offered [6].

The kinetics of molecular hydrogen accumulation at gamma radiolysis of water on the n- ZrO_2 surface is investigated. The influence of gamma radiations on n- ZrO_2 +water systems is studied at various temperatures T = 300...673 K [7].

In the temperature range $300 \le T \le 473$ K, the activation energy of the radiation-thermal process is 1.07 kJ/mol, and in the temperature range $573 \le T \le 673$ K, the activation energy of the thermal and radiation-thermal processes is 68.6 and 53.83 kJ/mol, respectively [8,9].

The amount, formation rate, and radiation-chemical yield of molecular hydrogen obtained from the water radiolysis



process within the system have been defined according to both water and BeO by maintaining the water volume constant (V = 5 ml); by changing the mass (mBeO = 0.0 (pure water), 0.01; 0.02; 0.04; 0.08; 0.2 g) and particle size (d < 4, d = 32...53 and 75...106 μ m) of beryllium oxide in the porous BeO/H₂O suspended systems by the influence of γ -quantum [10].

Photochemistry of water splitting

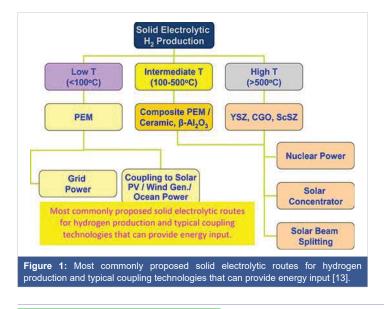
Herein, the primary systems prevent the spread of oxides as a result of the oxidation of hydrogen and remain relevant for use in high-pressure water-cooled reactors. The reunification of H_2 and H_2O_2 into water indicates the combination of H^+ ions and OH^{*} radicals. Under the influence of radiation, the chain reaction forms H^{*} and OH^{*} radicals at very low concentrations. Therefore, the breakdown of molecular hydrogen leads to the production of these compounds [11,12].

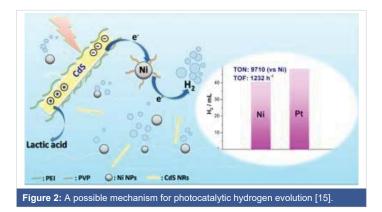
In heterogeneous systems, the process of water decomposition takes place in three stages. In these cases, the ways of energy reduction and energy transfer are subjected to ionizing radiation and physical and physicochemical reversible reactions. Thus, changes in the surface of nanoparticle oxide samples indicate the relevance of nanoparticles and are important for these physicochemical processes (Figure 1).

Energy transfer occurs during the adsorption process under the influence of high-energy radiation on the surface of nanoparticle oxide samples. These reactions can be considered "radiation catalysis". The production of molecular hydrogen in the process of radiolysis in the oxide-water system has been shown in numerous studies [13,14].

One of the main issues in conducting such research is the creation of new fuels and construction materials, and the discovery of new methods of material analysis control (Figure 2).

Nanostructures refer to macroscopic materials that contain nanoscale elements. The initial formation of atoms





with dimensions of $0.1 \div 1 \text{ nm} (10 \div 10^4)$ is observed in nanoclusters. Nanoparticles are usually used for small molecular nanoclusters with characteristic dimensions of atoms (molecules) to form intermediate products <100 nm [15-17].

If the properties of the clusters do not depend on the number of atoms, it can be assumed that a small amount of macroscopic material has been obtained. Examples of nanosystems smaller than 100 nm are clusters with 10 to 10^4 atoms. In two-dimensional objects, for example, nanostructures smaller than 100 nm, such as graphene and carbon nanotubes [18].

About 1% of the STE particles obtained are the values of the electron-hole centers. Many activities occur as a result of different STE groups and multiple interactions. The centers of the holes exposed to gamma radiation as a result of the processes have been studied by many scientists. The formation of an oxygen molecule as a result of the irradiation of metal samples is shown in this study. It is possible to show some of the mechanisms of obtaining a metal oxygen molecule as a result of radiation, which also exists as a result of reactions and is written in the form ("Me-O-O-Me") [19].

The monotony of the process must be broken in order to establish the kinetic parameters. The likelihood of encountering such cases usually occurs in rapid reactions. However, in this case, the situation becomes more complicated, when catalysts and inhibitors are used [20,21].

In oxide systems, it is almost more appropriate to obtain molecular hydrogen. Therefore, it is important to accelerate the decomposition reactions with free and pure water HO^{*}. In these systems, diffusion occurs in limited numbers between H₂ and HO^{*}. As a result of the positive effect of catalysts, diffusion coefficients are reduced. The photochemical water splitting to produce O₂ and H₂ is considered the most promising, sustainable, renewable, and cost-effective energy technology for the future. In the photochemical water splitting process, the efficiency of H₂ and O₂ production rates depend on the properties of the selected semiconductor material. However, most semiconductors face various limitations which confine their water-splitting efficiency. Different strategies could



be implemented to improve the water-splitting efficiency of semiconductors (Figure 3).

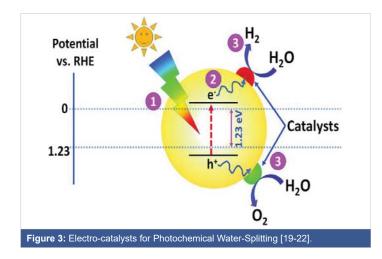
Among them, loading of catalyst onto the water-splitting material is known to be one of the effective strategies to enhance the H_2 and O_2 production rates. Given this, several catalytic materials have been explored and successfully utilized in efficient O_2 and H_2 production systems. The surface deposited catalysts were known to reduce the surface trap states, which decreases the charge recombination and acts as a protective layer to minimize photo-corrosion of the light-absorbing semiconductors. Conclusively, exploring the efficient catalysts for photochemical water splitting requires more research contribution toward the understanding of the core reaction mechanism of the catalytic process with the use of sustainable and stable materials.

Hydrogen production from water using a catalyst and solar energy is an ideal future fuel source. The search for suitable semiconductors as photo-catalysts for water splitting into molecular hydrogen and oxygen has been considered to be an urgent subject in our daily life. In this review, we aim to focus on the research efforts that have been made so far for H_2 generation from water splitting by UV and visible-lightdriven photo-catalysis. A number of synthetic modification methods for adapting the electronic structure to enhance the charge separation in photo-catalyst materials are discussed. Sacrificial reagents and electron mediators for the overall water splitting are also reviewed. The quantum efficiency of photo-catalyst materials upon visible and UV illumination will be reviewed, summarized and discussed [22].

Importance of radiations in hydrogen generation

UV radiation: In the past, manufacturers' labeling of sunscreen varied greatly, confusing consumers regarding the efficacy and the appropriate photoprotection provided by their products (Figure 4).

This article discusses ultraviolet radiation and the positive and negative effects of ultraviolet radiation provides a review of sunscreens and discusses the new regulations for



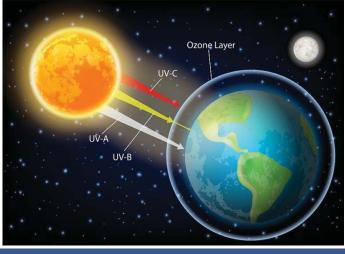


Figure 4: The ultraviolet component of the electromagnetic spectrum [23,24].

sunscreens of the United States Food and Drug Administration (FDA) [23,24].

Visible radiation: Energy radiated in the visible part of the spectrum of various oxides and their mixtures when heated to red brightness temperatures between 1400 and 2000K by means of cathode-ray bombardment, and gasair and oxy-gas flames were measured by an optical pyrometric method. [25,26]. The energy of this radiation must be captured as excited electron-hole pairs in a semiconductor, a dye, or a chromophore, or as heat in a thermal storage medium (Figure 5).

Materials, for thermal applications, have optical properties that make them well adapted for utilizing solar energy and for reaching energy efficiency, especially in the built environment [27].

Gamma radiation: The kinetics of molecular hydrogen accumulation at gamma radiolysis of water on n-MeOsurface is investigated. The influence of gamma radiations on n-MeO+water systems are studied at various temperatures (Table 1) T = 373...673 K. [28-32].

It is found that n-MeO displays radiation-catalytic activity in the decomposition of hexane and hexane–water mixture, as a result of which the rate of accumulation of molecular hydrogen increases (Figures 6,7).

These results are promising for molecular hydrogen generation by water splitting in near future [33,34].

X-ray radiation: It is desirable that the employed catalyst is nano-sized and disperses throughout the system to increase catalyzing efficiency [35-39].

The formation of radiolytic (Figure 8) products such as H_2 or H_2O_2 has to be evaluated for safety reasons, in order to prevent the breaking or the corrosion of the confining matrix [40-44].



Neutron radiation: Hydrogen saturation of titaniumbased materials exposed to irradiation with resonance neutrons with an energy of 0.1 MeV is considered [44,45] (Figure 9).

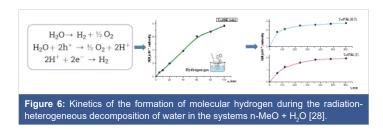
Shielding neutrons involve three steps that are slowing neutrons, absorption of neutrons, and impregnation of gamma rays. Neutrons slow down with thermal energy by hydrogen, water, paraffin and plastic. Hydrogenated materials are also very effective for the absorption of neutrons [46].

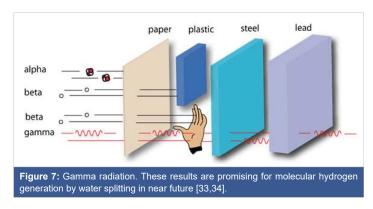


Figure 5: The different ways of utilizing the energy coming from solar and ultravio irradiation [26,27].

Table 1: The value of the rates and radiation-chemical yields of molecular hydrogen during radiation-thermal, thermal and radiation processes of water decomposition in the n-ZrO₂+H₂Oabs. The system at different temperatures with different particle sizes.

Particle size d, nm	W _{RT} (H₂), molecules/g·s	W _⊤ (H₂), molecules/g·s	W _R (H₂), molecules/g·s	G(H₂), molecules/100eV
20-30	9,17 · 10 ¹³	1,38 · 10 ¹³	7,8 · 10 ¹³	4,8
	2,08 · 10 ¹⁴	0,56 · 10 ¹⁴	1,52 · 10 ¹⁴	8,35
	3,33 · 10 ¹⁴	1,11 · 10 ¹⁴	2,22 · 10 ¹⁴	13,6
	6,94 · 10 ¹⁴	2,78 · 10 ¹⁴	4,16 · 10 ¹⁴	25,7
50-70	7,88 · 10 ¹³	2,5 · 10 ¹³	5,28 · 10 ¹³	3,3
	1,5 · 10 ¹⁴	0,5 · 10 ¹⁴	1,0 · 10 ¹⁴	6,2
	2,78 · 10 ¹⁴	0,83 · 10 ¹⁴	1,95 · 10 ¹⁴	10,4
	5,14 · 10 ¹⁴	2,08 · 10 ¹⁴	3,06 · 10 ¹⁴	19,6





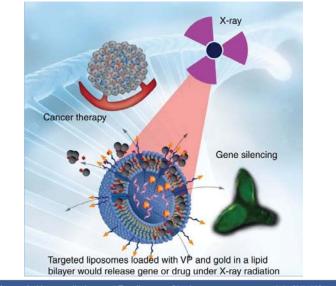
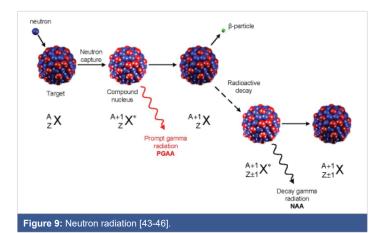


Figure 8: X-ray radiation and Family tree of hydrogen storage materials [35-40].



Mechanism of radiation in hydrogen generation

Electrons generated by radiation inside a nanoparticle of radius R suspense in fluid water are diffused with equal probability in all directions inside the particle and gradually lose their kinetic energy as a result of elastic and inelastic collisions. Some of these electrons are transported to the nanoparticle surface during the physical and physicochemical stages of the process and emitted into the water. Using the Monte Carlo, step-by-step, single-collision methods, the trajectories of electrons were tracked based on the Mathcad program and the percentage of electron emissions from the nanoparticle surface into the water was calculated. It was found from the calculations that the emission percentage changes depending on the size of the nanoparticle and the energy of the electrons [47-51].

Future perspective of radiations role in hydrogen generation

Herein in this review, the results of exploring the prospects of the hydrogen economy are presented. It is shown that the comparative analysis of the economic competitiveness of these chains with each other with solutions based on the use



of alternative fuels has been performed, respectively. The analysis has established the most promising directions in the development of the hydrogen economy in order to justify the economical value of this research.

Conclusion

The monitoring of different radiation-induced changes in the surface and the choice of the performance characteristic of a heat-resistant catalytic material based on these nanomaterials. Thus, in this way, the base of nanomaterials' radiation-catalytic processes enables the transformation of ionizing radiation energy to chemical one with great efficiency. Radiation-heterogeneous systems with nano-size open a new actual direction in radiation processes and the radiative study of materials. It is clear from the presented results that nanostructured materials become an important role in nuclear-power engineering as structural and functional materials practically in all stages of the nuclear fuel cycle. It is extremely important for the formation of nanostructured materials after exposure to ordered nanostructure from the new phase with a period of a few nanometers, promoting the preservation of the properties of materials under high irradiation.

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