Advanced Physical Research
Vol.4, No.2, 2022, pp.106-110

INFLUENCE OF NEUTRON FLUX ON THE CRYSTAL STRUCTURE OF Y_2O_3 NANOPARTICLES

R.F. Rzayev*

Azerbaijan State Pedagogical University, Baku, Azerbaijan

Abstract. The influence of the neutron flux on the crystal structure of Y_2O_3 nanoparticles has been studied. Yttrium oxide nanoparticles with a size of d = 20-40 nm were irradiated with neutrons with an energy of E < 1 MeV to an intensity of I < 1015 n/cm². Structural studies were carried out by X-ray diffraction method. It has been established that the crystal structure of Y_2O_3 nanoparticles corresponds to cubic symmetry with space group Ia-3. The highly symmetrical crystal structure did not change upon irradiation. An additional background appeared in the X-ray diffraction spectra, which was partly explained by amorphization. The mechanism for changing the values of the lattice parameters depending on the intensity of neutron radiation is determined.

Keywords: *Yttrium oxide, neutron radiation, crystal structure, X-ray diffraction analysis.*

Corresponding Author: *R.F. Rzayev, Azerbaijan State Pedagogical University, AZ-1000, Baku, Azerbaijan, e-mail: ravilrzayev@mail.ru*

Received: *13 June 2022;* ***Accepted:*** *22 July 2022;* ***Published:*** *30 August 2022.*

1. Introduction

The Y_2O_3 compound is one of the most widely studied compounds among nanomaterials (Wang *et al.*, 2009; Hua *et al.*, 2017). It is known that rare earth elements are elements that impart optically active properties to materials. Therefore, compounds formed by these elements and matrix materials included in the form of additives exhibit interesting physical properties (Leanenia *et al.*, 2015; Tagiyev *et al.*, 2015; Leanenia *et al.*, 2017). It is impossible to explain the mechanism of formation of many physical properties in complex compounds. Therefore, it is expedient to use simple materials as model objects for research. For this purpose, the Y_2O_3 nanocompound can be considered the most suitable model object.

The Y_2O_3 compound is a compound with interesting structural properties despite its simple chemical form. It was found that this compound can have two different crystal structures (Guo *et al.*, 2006; Baldinozzi *et al.*, 1998; Ferreira *et al.*, 2005). Each of these modifications was studied by XRD at room temperature. As can be seen from the analysis of the obtained diffraction patterns, the diffraction pattern of the first modification corresponds to the cubic syngony. The space group of this phase corresponds to the space group of high symmetry Ia-3. The diffraction pattern of the second modification of yttrium oxide corresponds to monoclinic syngoniasis. This phase corresponds to the space group C2/m (Baldinozzi *et al.*, 1998). It has been established that the crystal structure of the yttrium oxide compound depends on the conditions of synthesis of this material. In the course of theoretical studies carried out in the temperature range T = 0-1500 ºC and pressure range P = 0-60 GPa, it was found that in addition to the cubic and monoclinic phases, it is possible to obtain one more modification corresponding to the hexagonal

phase. Although the cubic phase exists under normal conditions, at pressures $P > 15$ GPa the symmetry of the crystal structure decreases and a monoclinic phase exists. At pressures $P > 50$ GPa, the symmetry of the crystal structure begins to increase again and a hexagonal phase is present (Razavi-Khosroshahi *et al.*, 2017).

In addition to the investigation of the crystal structure of the Y_2O_3 compound, the surface structure and size effects have also been investigated. SEM images of the Y_2O_3 compound at a scale of ~200 nm under normal conditions and at room temperature show that the nanoparticle sizes are smaller in the cubic modification. In the monoclinic modification, the sizes of nanoparticles are larger compared to the cubic modification and can reach $d \approx 100$ nm. This is due to the fact that as the symmetry of the structure increases, densification of materials is possible. Therefore, it was possible to obtain nanoparticles of a smaller volume in a highly symmetrical modification.

An atomic force microscope (AFM) is one of the methods used to study the structural properties of nanomaterials. In these microscopes, the surface structure and surface histograms of nanomaterials obtained in the form of thin layers are studied. The morphology of thin layers of yttrium oxide has also been studied. It was found that the crystal structure of the yttrium oxide compound significantly affects the size of the nanoparticles. Based on the surface structure, taken on a scale of d ~ 2 μm, it was determined that the size of nanoparticles with monoclinic symmetry is 2 times larger than the size of nanoparticles with cubic symmetry.

As a result of complex structural studies of yttrium oxide nanomaterials using X-ray diffraction, scanning electron microscope and atomic force microscope, it was found that yttrium oxide nanoparticles can have different symmetry due to their crystal and surface structure. It is known that the size of nanoparticles affects not only their structural properties. It also affects the optical and electrical properties. Although the structural properties of yttrium oxide nanoparticles have been studied, the effect of ionizing radiation on these properties has not been studied. In this work, we studied the effect of a high-intensity neutron beam on the crystal structure of yttrium nanoparticles.

2. Experimens

In this work, we study the effect of a neutron beam on the crystal structure of a nanosized Y_2O_3 compound. The objects of study were irradiated with a neutron flux of various intensities in the IBR-2M reactor located in Dubna, Russia (Mirzayev *et al.*, 2021; Miyazawa *et al.*, 2020; Mirzayev *et al.*, 2021). The structural properties of unirradiated and irradiated samples with a high-intensity neutron flux at room temperature and under normal conditions were studied by X-ray diffraction. The experiments were performed on a D8 Advance diffractometer (Bruker, Germany) with parameters of 40 kV, 40 mA, $\lambda = 1.5406$ Å, CuKα radiation. The results obtained were analyzed by the Rietveld method in the Fullprof program and using the Gaussian function in the Origin program.

3. Results and Discussion

When studying the structural properties of Y_2O_3 nanoparticles, their surface structure and size effect were studied for the first time. In the course of studies carried out on a scanning electron microscope at a scale of 100 nm, it was found that the size of nanoparticles in the form of rubbing varies in the range $d = 20–40$ nm. It is known that the properties of materials change at the nanoscale ($d = 1$-100 nm). Therefore, it is

important to find materials capable of maintaining nanosizes for a long time and to study their physicochemical properties. It has been established from previous studies that yttrium oxide nanoparticles are a stable material in this regard and retain their nanosize for a long time. These properties indicate oxidation, decomposition, formation of hydroxide groups due to combination with water molecules, etc. in the material. this is due to the absence of such physicochemical processes.

The crystal structure of yttrium oxide nanoparticles was studied by X-ray method at room temperature. The resulting radiograph is shown in Fig. 1.

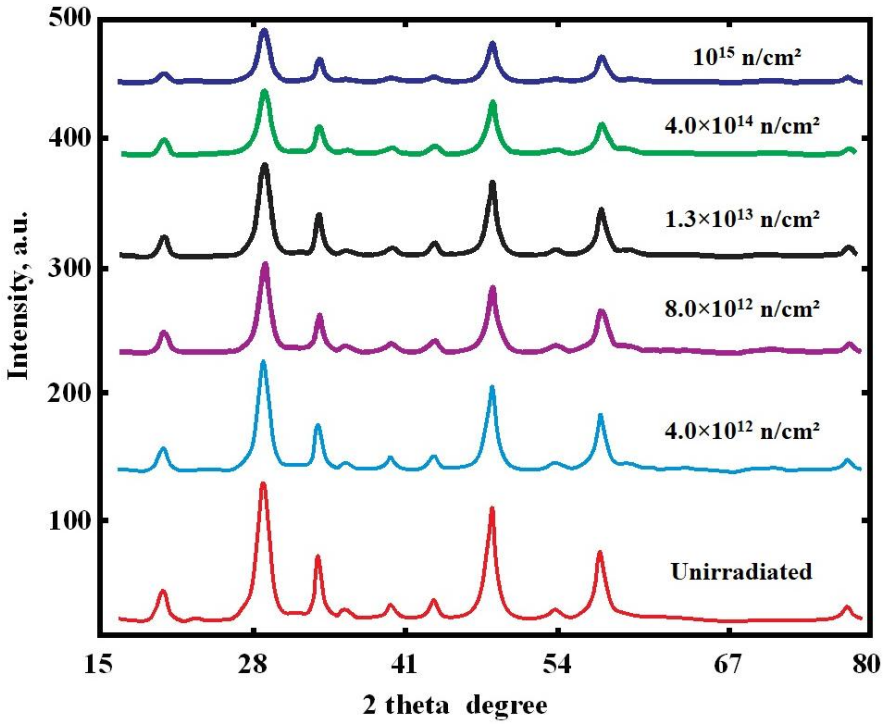

Fig. 1. X-ray diffraction spectra of Y_2O_3 nanoparticles irradiated with an intensity of 4.0×10^{12} n/cm², 8.0×10^{12} n/cm², 1.3×10^{13} n/cm², 4.0×10^{14} n/cm² and 10^{15} n/cm² cm²

When analyzing the spectrum, it was found that the crystal structure of the Y_2O_3 compound has cubic symmetry with a highly symmetrical space group Ia-3. Values of unit cell parameters: $a = b = c = 10.5958$ Å. In the analysis by the Rietveld method, it was found that the trivalent yttrium atoms are in two different positions in the crystal lattice. The first yttrium atom (Y1) is at coordinates $x = 1/4$, $y = 1/4$ and $z = 1/4$, the second yttrium atom (Y2) is at coordinates $x = -0.0165$, $y = 0$ and z = 1/4. Divalent oxygen atoms are located in the same position: coordinates $x = 0.3942$, $y = 0.1428$ and $z = 0.3825$. Oxygen atoms form various bonds with yttrium atoms in the range $d_{O\text{-}Y} = 2.1628\text{-}2.4083$ Å. Of great importance is the length of bonds between atoms of the same element. The interval contains bonds between oxygen atoms: $d_{O\text{-}O} = 2.8207\text{-}3.7003$ Å and bonds between yttrium atoms: $d_{Y\text{-}Y} = 3.6416\text{-}3.8922$ Å.

Bonds between oxygen atoms: $d_{O\text{-}O} = 2.8207\text{-}3.7003$ Å, bonds between yttrium atoms: $d_{Y\text{-}Y} = 3.6416\text{-}3.8922$ Å, are located in the interval. When we compare the values of interatomic distances, we see that as the ionic radii increase, the atoms are located at a greater distance from each other. Therefore, there are some differences in the lengths of

the bonds they form. It is known that the ionic radii of oxygen atoms, which are considered light elements, are smaller. Rare earth yttrium atoms, which are considered heavy elements, have larger ionic radii than oxygen atoms. When the electrons leaving the yttrium, element form a covalent bond, they fill the outer electron shell of the oxygen atom. Consequently, the ionic radii of oxygen atoms are larger in the case of divalent. For this reason, oxygen-oxygen bonds are larger than oxygen-yttrium bonds.

The effect of a neutron beam on the crystal structure of Y_2O_3 nanoparticles has been studied. d = 20-40 nm nanoparticles of yttrium oxide compound irradiated with neutrons with energy E < 1 MeV. Irradiation was performed at 5 different intensities: 4.0×10^{12} n/cm², 8.0×10^{12} n/cm², 1.3×10^{13} n/cm², 4.0×10^{14} n/cm² and 10^{15} n/cm². After irradiation, the crystal structure of the samples was studied by the X-ray method, the obtained spectra were compared with the X-ray diffraction spectrum of the unirradiated sample. The X-ray diffraction spectra obtained at room temperature for Y2O3 nanoparticles irradiated with different intensities are shown in Fig. 1. It has been established that there are no fundamental changes in the crystal structure of the samples upon irradiation with the indicated intensities. When analyzed by the Rietveld method, it was found that the crystal structures correspond to cubic symmetry with the space group Ia-3.

4. Conclusions

When comparing the spectra, two main effects were observed:

1. As the radiation intensity increased, the peaks in the X-ray patterns shifted to the right along the abscissa axis. This effect is a sign of an increase in interatomic distances and a corresponding increase in the lattice parameters. It is known that when irradiated with high-energy neutrons, weak bonds in crystals, including nanoparticles, break, and therefore some bonds expand. These expansions are reflected in radiographs.

2. As the radiation intensity increased, a decrease in the intensity of the peaks in the X-ray patterns was observed, and an additional background began to form. This effect is explained by the initiation of partial amorphization due to the breaking of some weak bonds in crystals, including nanoparticles, upon irradiation with high-energy neutrons.

When studying the crystal structure of yttrium oxide nanoparticles irradiated with neutrons with energy E < 1 MeV to intensity I < 1015 n/cm², it was found that these particles have a fairly stable action before neutron irradiation. Despite the breaking of some weak bonds during collisions of high-intensity beams with nanoparticles, in general, nanoparticles retain their structural properties and retain a highly symmetrical crystal structure.

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