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Influence of a neutron beam on the electrical properties of nanosized Y_2O_3 crystals

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Abstract

In the presented work, high purity yttrium oxide (99.99%), nanosized crystal density 0.069 g/cm^3, specific surface area 100-150 m^2/g, average crystal size 8-10 nm and difrent intensities (4.0×10^{12} n/cm^2 , 1.3×10^{13} n/cm² and 4.0×10^{14} n/cm²) in the temperature range of 300-700 K, the electrical properties were investigated after irradiation with fast neutrons. It has been established that the electrical properties of Y_2O_3 nanocrystals in a wide temperature range show an increase in the electrical conductivity according to a linear law after irradiation of various intensities. The increase in conductivity depending on the intensity of fast neutron radiation is due to the predominance of yttrium vacancies in the conductivity.

Keywords: yttrium oxide nanocrystal, electrical conductivity, fast neutrons, activation energy.

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1. Introduction

Although oxide materials have a simple chemical form, they have different physical properties. They are ferroelectric, ferromagnetic, and other properties are observed [1-5]. Therefore, these materials are widely studied. As a result of these studies, the possibilities of technical application of oxide materials are expanding [6-10]. Recently, size effects in functional materials have been widely studied. It has been established that the properties of materials change depending on the size of crystallites and particles [11-15]. The main studies carried out in this direction relate to nanomaterials [16-20].

In recent years, the structural properties of Y_2O_3 nanocrystals after irradiation with various radiation sources have been widely studied in experimental studies of nanomaterials and nanosized crystals [21,22]. Composite compounds formed by a Y_2O_3 nanocrystal with oxide and ceramic materials such as ZrO_2, SiO_2, TiC, ZrC in various concentrations were studied by analytical methods [23,24]. It is known that samples of Y_2O_3 nanocrystals have high thermal and electrical conductivity and high mechanical properties. High thermophysical properties and the absence of oxidation and structural destruction in a wide temperature range are studied more from a thermal point of view [25]. However, it was established by theoretical calculations that it is very important to study the electrical conductivity of samples with the Y_2O_3 structure [26]. From room temperature to 1000 K, the thermal conductivity of the Y_2O_3 sample changes according to a decreasing law [27,28]. In studies carried out on the electronic structure of Y_2O_3 in various media, the fundamentals of the electronic configuration of O and Y atoms, changes in the electron density and electron exchange upon interaction with various compounds were studied [29]. It is known that structural changes upon irradiation with fast neutrons affect the mechanical, electrical, and thermal properties of nanocrystals [30]. The effect of a neutron beam on many properties of yttrium oxide has been studied. However, the influence of the neutron beam on the electrical properties has not been studied.

The electrical properties of yttrium oxide nanoparticles after irradiation with fast neutrons with an energy of 1 MeV have been studied and the activation energy of nanoparticles has been determined.

2. Experiments

In the presented work, yttrium oxide crystals of high purity (99.99%), density of nanosized crystals 0.069 g/cm^3, specific surface area 100-150 m^2/g, and average crystal size 8-10 nm were studied. Samples for research were irradiated at room temperature with fast neutrons with an energy of 1 MeV, a flux density of 4.0×10^{12} n/cm², 1.3×10^{13} n/cm² and 4.0×10^{14} n/cm² in the IBR-2M reactor of the Laboratory of Neutron Physics Joint Institute for Nuclear Research. When studying the electrical properties of nanocrystals, samples were prepared, especially those with a quadrangular shape, the surfaces of the anode and cathode were polished, and the resistivity was experimentally measured. When measuring electrical properties, electrodes, thermocouples, a heating furnace, a current source, and a voltmeter were used. After placing the nanocrystals between the electrodes, linear heating was carried out with a heater at a rate of 2.5 deg/min. The sample temperature is measured by a thermocouple, and its resistance by an E6-13A thermometer. Using the experimental values obtained from the temperature dependence of the electrical conductivity, the value of the activation energy was calculated. The activation energy was determined in Arenius coordinates.

3. Results and discussion

Samples of Y_2O_3 nanocrystals were fabricated in the form of a parallelepiped geometric shape by pressing; the effect of irradiation with fast neutrons on electrical conductivity in the temperature range of 290-630 K was studied. Changes in defects formed under the action of radiation under the action of an electric field and the effect of vacancies formed in the structure on electrical conductivity were studied. Before irradiation, nanocrystalline samples were subjected to heat treatment at a temperature of 1300 K. After the heat treatment process, the initial values of the radiation of the samples were measured. Experimental measurements were carried out at a constant value of the electric field of 12 V. An E3-13A device was used to study the resistance of the samples as a function of temperature. The given areas of nanocrystals, the distance between the contacts, and the electrical conductivity of this material were determined from the resistance using a certain specific resistance. On Figure 1 shows the temperature dependence of the electrical conductivity of a Y_2O_3 nanocrystal irradiated with fast neutrons of various intensities up to a temperature of 700 K. It is determined that crystals with a highly active surface do not affect the electrical conductivity of water molecules with a weak chemical interaction with the surface in the temperature range of 290-630 K. Y_2O_3 is a semiconductor with a band gap of 5.6 eV, which changes its electrical conductivity by small values over a wide temperature range.

It was found that the electrical conductivity of unirradiated samples of Y_2O_3 nanocrystals varies linearly in the temperature range 290-630 K. An increase in the intensity of the fast neutron flux led to an increase in the electrical conductivity in a given temperature range. To determine the electrical conductivity mechanism, the electrical conductivity of unirradiated samples of Y_2O_3 nanocrystals was re-measured under repeated measurement conditions. Studies carried out by the method of "Differential scanning calorimetry" showed that on the surface of samples of Y_2O_3 nanocrystals in the temperature range of 300-540 K, a complex process occurs, such as dehydration of weakly absorbed water molecules. The kinetics of the dehydration process as a mechanism makes it possible to give a numerical value of electrical conductivity, to reveal patterns in a wide temperature range, and also to make assumptions about the general change in electrical conductivity depending on the intensity flux of fast neutrons. Water molecules absorbed on the active surface of nanostructured compounds form an ion-dipole interaction with cations in the bulk, and as a result of this interaction, new hydroxyl functional groups are formed.

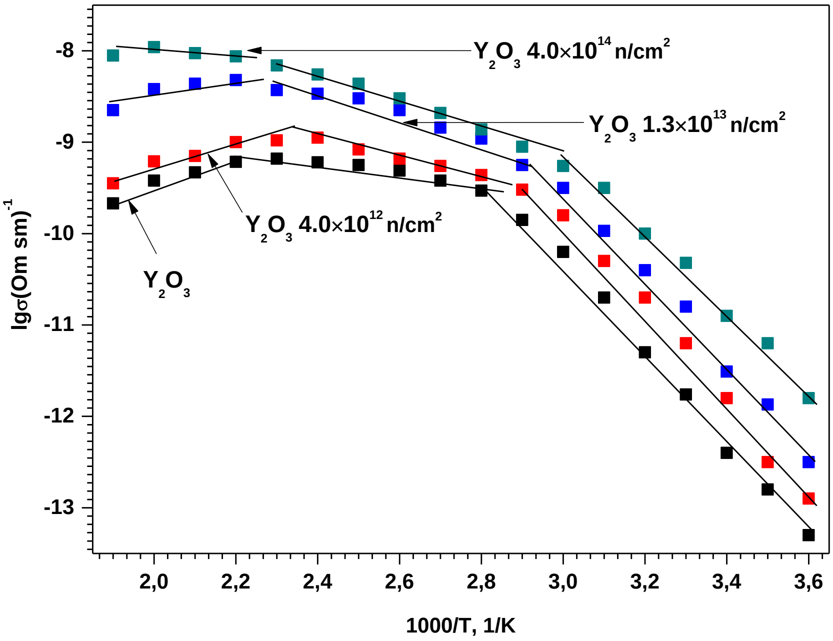

Figure 1. Temperature dependence of the electrical conductivity of a Y_2O_3 nanocrystal unirradiated and irradiated with fast neutrons of various intensities.

The mechanism of desorption of water molecules on the crystal surface is in the nature of anions and cations Y and O in the electrical conductivity of the sample. As the intensity of the fast neutron flux increases, the observed changes in the electrophysical properties can be explained by the activation of vacancies, point defects, and excited states. Charged and structural defects are formed under the action of neutron beams on nanocrystals. The mechanism for the formation of electric carriers can be represented as follows:

$$Y_2O_3 \rightarrow e^+,\ e^-,\ S^*, \equiv Y, \equiv YO$$

Here e^+, e^- are hole and electron unbalanced charge carriers, S^* is an active adsorption center, ≡YO and ≡Y are formed radical states. The resulting nonequilibrium charge carriers occupy positions in electron donor and electron acceptor vacancies in the structure. It represents localized states of localized centers and nonequilibrium charge carriers in donor and acceptor states of electrons. For the participation of electric charge carriers in the process of electrical conduction, an external energy transition is necessary in order to occupy the vacant place of localization centers. It is from this aspect that the case of a linear increase in the electrical conductivity after 460 K takes place. In the samples of Y_2O_3 nanocrystals irradiated with neutrons, the change with temperature indicates the formation of a cascade of homogeneous defects in this region.

It has been found that the electrical conductivity of Y_2O_3 nanocrystal samples in the temperature range of 300-600 K and the activation energy of the process are composed of several parts. The influence of irradiation on the activation energy of electrical conductivity in a wide temperature range is shown in Table. With an increase in the activation energy, depending on the temperature, the activation of the centers of the energy barrier occurred. An increase in the radiation intensity of the fast neutron flux caused a decrease in the activation energy. The value of the activation energy in non-irradiated samples was 4.32, 2.23 and 1.04 eV depending on the temperature intervals, which is consistent with the activation energies of vacancies and point defects.

Intensity	**Activation energy, eV**		
	280-330 K	**330-420 K**	**420-530 K**
Non-irradiated sample	4.32	2.23	1.04
4.0×10^{12} n/cm^2	4.30	2.20	1.02
1.3×10^{13} n/cm^2	4.28	2.15	1.00
4.0×10^{14} n/cm^2	4.16	2.09	0.8

Table. Activation energy of Y_2O_3 nanoparticles irradiated with neutrons

As can be seen from the values given in Table, the activation energy decreased as the radiation intensity increased. This is due to the fact that additional charge carriers were created by exposure to ionizing radiation.

4. Conclusion

Samples of Y_2O_3 nanocrystals irradiated with fast neutrons of various intensities 4.0×10^{12} n/cm^2, 1.3×10^{13} n/cm^2 and 4.0×10^{14} n/cm^2 (purity 99.99%, powder density 0.069 g/cm^3, specific surface 100-150 m^2/g, particle size 8-10 nm) electrical conductivity was studied in the temperature range $280 \leq T \leq 530$ K. It was determined that the value of electrical conductivity in a given temperature range varies from log(-13) to log(-8) when separating different parts. The value of activation energy at intensities of 4.0×10^{12} n/cm^2, 1.3×10^{13} n/cm^2 and 4.0×10^{14} n/cm^2 was 4.30, 4.28 and 4.16 eV. For the first time, the mechanism of electrical conductivity caused by ionizing radiation in yttrium oxide nanoparticles has been established.

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