SYNTHESIS OF COMPLEX OXIDE $La_{0.5}Ba_{0.5}MnO_3$ AND STUDY OF ITS SIZE EFFECT

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Abstract: In this work, the complex oxide $La_{0.5}Ba_{0.5}MnO_3$, which is a perovskite-type compound, was synthesized. Preliminary analyzes of the resulting sample were carried out. The crystal structure has been determined. Covalent bonds formed by metal and oxygen atoms were analyzed. The crystal structure is explained by MnO_6 octahedra. The effects that occur during cation-cation substitutions are indicated. To study the size effect, studies were carried out under an SEM microscope. Based on the surface structure obtained at different scales, it was determined that the crystallite sizes are on the order of microns.

Keywords: oxide, covalent bond, crystal structure, morphology.

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Introduction:

Recently, oxide materials have been widely studied. The main reason for the interest of these materials is that their chemical composition is stable over a long period of time. Because oxidation occurs on the surface of non-oxide materials. Therefore, changes in their chemical composition are observed after a certain period of time. Complex oxides are considered more interesting objects. In these compounds, piezoelectric, ferroelectric and other properties are observed. It is known from the chemistry of semiconductors that these compounds also have semiconducting properties (Heywang, 1971; Karpierz & ets, 2017; Yousaf Shah & ets, 2020; Fujioka & ets, 2001; Razak & ets, 2017).

It has been established that when metal atoms, such as Fe, Ni, and Co, are included in the composition of complex oxides, magnetic properties are also observed in these materials. Therefore, by changing the chemical composition of these oxides, materials with different functions can be synthesized. Ferro- and antiferromagnetic properties were observed in the compounds $BiMnO_3$, $BiFeO_3$, $BaMnO_3$ (Dash & ets, 2016; Haykal & ets, 2020; Sosnowska & ets, 1995; Chamberland & ets, 1970). To obtain new functions in these chemical compounds, it is necessary to study their physicochemical properties. It has been established that the physical properties of barium hexaferrite and its solid solutions are affected by their size. Therefore, the size effect was studied in these compositions. In studies carried out using a scanning electron microscope, it was found that the size effect also changes depending on the concentration of chemical elements in the composition (Trukhanov & ets, 2016; Ayyubova, 2021). As the concentration of magnetic ions in complex oxides increases, the crystallite size increases. This effect is associated with the formation of long-range magnetic order.

The information obtained about the surface structure of chemical compounds allows us to obtain information about a number of properties of these compounds. Therefore, it is important to study their size effect in the preparation of nanoparticles and thin films, as well as their physicochemical properties.

Although a number of chemical properties of the $La_{0.5}Ba_{0.5}MnO_3$ compound have been studied, its size effects have not been sufficiently studied. In this work, polycrystals of the $La_{0.5}Ba_{0.5}MnO_3$ compound were synthesized and a structural-phase analysis of the resulting composition was carried out. The size effect of the resulting compound was studied using a scanning electron microscope. Size effects were studied using data obtained from surface structures obtained at the *D* = 10 μm and *D* = 1 μm scales. It has been established that, based on images obtained at different scales, it is possible to obtain information about the acquisition of polycrystals, the shape, size and degree of crystallization of crystallites.

Experiments:

The compound $La_{0.5}Ba_{0.5}MnO_3$ was obtained by chemical reactions using a procedure consisting of several stages. The reaction involved oxides La_2O_3, Mn_2O_3 and $BaCO_3$ of high purity (>99.999%). Based on the conditions of the chemical reaction, it was taken based on the molar mass of these oxides. La_2O_3 oxide was heated in open air at a temperature of 1000 °C for 2 hours, water and carbon dioxide molecules were removed from its composition. At the next stage, the oxides were mixed in the appropriate amount and pressed to a size of 20 mm. The material prepared in this way was heated in the open air for 5 hours at a temperature of 1000 °C until the barium carbonate completely decomposed. In the next step, the sample was again ground in a mortar and mixed with the powder. At the final stage, the sample was placed on a platinum substrate and heated in open air at a temperature of 1550 °C for 10 hours. After the synthesis process, the sample was cooled at a rate of 80 °C per hour.

An X-ray phase analysis of the sample obtained after the synthesis process was carried out. The structural phase analysis of the obtained samples was carried out by X-ray diffraction (D8 Advance, Bruker, Germany). Diffractometer parameters: 40 kV, 40 mA, CuKα – radiation, λ = 1.5406 Å. The experiments were carried out at room temperature. During the structural analysis of the $La_{0.5}Ba_{0.5}MnO_3$ solid solution, it was established that a single-phase compound was synthesized.

The surface structure and size effects of chemical compounds were studied using a scanning electron microscope. Experiments were carried out on SEM, ZEISS, ΣIGMA VP instruments. Data on polycrystalline compounds $La_{0.5}Ba_{0.5}MnO_3$ were obtained by analyzing images taken at different scales.

Results and discussion:

The morphology and crystal structure of polycrystals of the La0.5Ba0.5MnO3 compound have been studied. X-ray phase analysis established that the crystal structure of this compound corresponds to the Fm-3m space group and cubic system. The lattice parameter values are set to a = b = c = 3.9073 Å. Since this crystal structure has high symmetry, it is also used as a model object in solving a number of problems. This structure is suitable for studying the formation of covalent bonds in crystallography and the influence of ionic radii on the structure. It is known that the elements lanthanum and barium alternately participate in this chemical compound. The high symmetry of the crystal structure of the resulting compound indicates that the barium and lanthanum atoms in this compound can completely replace each other. Therefore, the synthesis and study of the structure of the $La_{0.5}Ba_{0.5}MnO_3$ compound are useful not only for studying the size effect that occurs in complex oxides, but also for studying cation-cation substitutions in these compositions. MnO_6 octahedra are formed when Mn atoms in this composition form covalent bonds with O atoms. Depending on the position of these octahedra in the crystal, physicochemical properties are formed. When the atoms forming the octahedron are arranged in ideal coordinates, the Mn atoms located at the center of the octahedron form long-range magnetic order. In this case, magnetic properties are formed. Ba and La atoms form the perovskite structure, standing at the sites of the elementary lattice. The results obtained from studying the structure of the $La_{0.5}Ba_{0.5}MnO_3$ compound have important scientific significance both for explaining other properties of this compound and for explaining a number of properties inherent in complex oxides. Because the main structural elements in complex oxides are polyhedra. Perovskites consist mainly of octahedra. In hexaferrites there are tetrahedra, bipyramids and octahedra. Therefore, to explain the processes occurring in oxide materials, it is necessary to study polyhedra formed on the basis of covalent bonds formed in them by divalent oxygen atoms.

Structural analysis shows that the compound $La_{0.5}Ba_{0.5}MnO_3$ has interesting properties. Therefore, it is important to study other properties of this composition. It is known that the study of surface structure, as well as crystal structure, allows one to obtain extensive information about materials. Due to the fact that partial oxidation occurs on the surface of non-oxide materials, the data obtained are not sufficient to obtain accurate information. However, oxidation on the surface of oxide materials is minimal. Therefore, studying the surface processes occurring in them allows one to obtain accurate results. For this purpose, the morphology of the $La_{0.5}Ba_{0.5}MnO_3$ compound was studied. The surface structure obtained using a scanning electron microscope is shown in Figure 1.

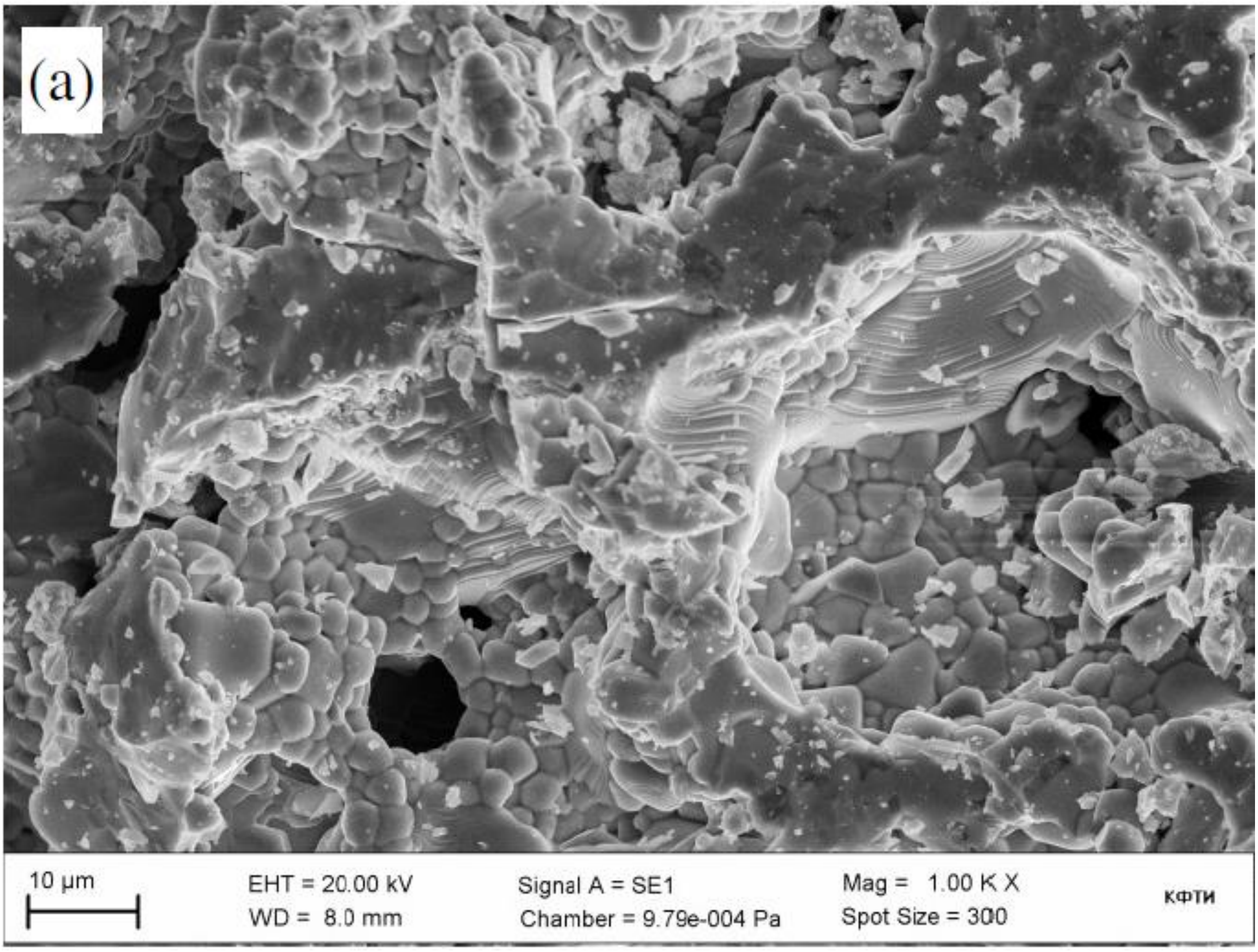

Figure 1. Surface structure of the $La_{0.5}Ba_{0.5}MnO_3$ compound on a scale of *D* = 10 µm.

From the surface structure shown in Fig. 1, it can be seen that the compound $La_{0.5}Ba_{0.5}MnO_3$ was synthesized in polycrystalline form. Despite the presence of voids in some parts, in general the distances between crystallites are very small. Obtaining samples depends on the synthesis conditions and technology. However, the formation of physicochemical properties is possible depending on the elements included in the chemical composition and the nature of the material.

The magnetic properties of materials also affect the formation of crystallites. Because magnetic domains are also formed in these crystallites. In materials with ferroelectric properties, domains are formed in crystallites as a result of the polarization process. From Figure 1 it can be seen that the crystallite sizes are on the order of microns. However, it is impossible to determine the exact dimensions.

In the $La_{0.5}Ba_{0.5}MnO_3$ compound, smaller size studies were carried out in order to more accurately determine the crystallite size and determine the size effect. In order to study the surface structure of the $La_{0.5}Ba_{0.5}MnO_3$ compound on a scale of D = 1 µm, studies were carried out using a scanning electron microscope. The results obtained are shown in Figure 2. From the surface structure shown in Figure 2, it can be seen that the $La_{0.5}Ba_{0.5}MnO_3$ compound was synthesized in the form of a high-density polycrystal. In small sizes there are almost no gaps in this composition. It was determined that the crystallite size is in the range D = 1-3 µm. In some parts this composition was observed in layered form, which is an indication of the smaller crystallite sizes in these parts.

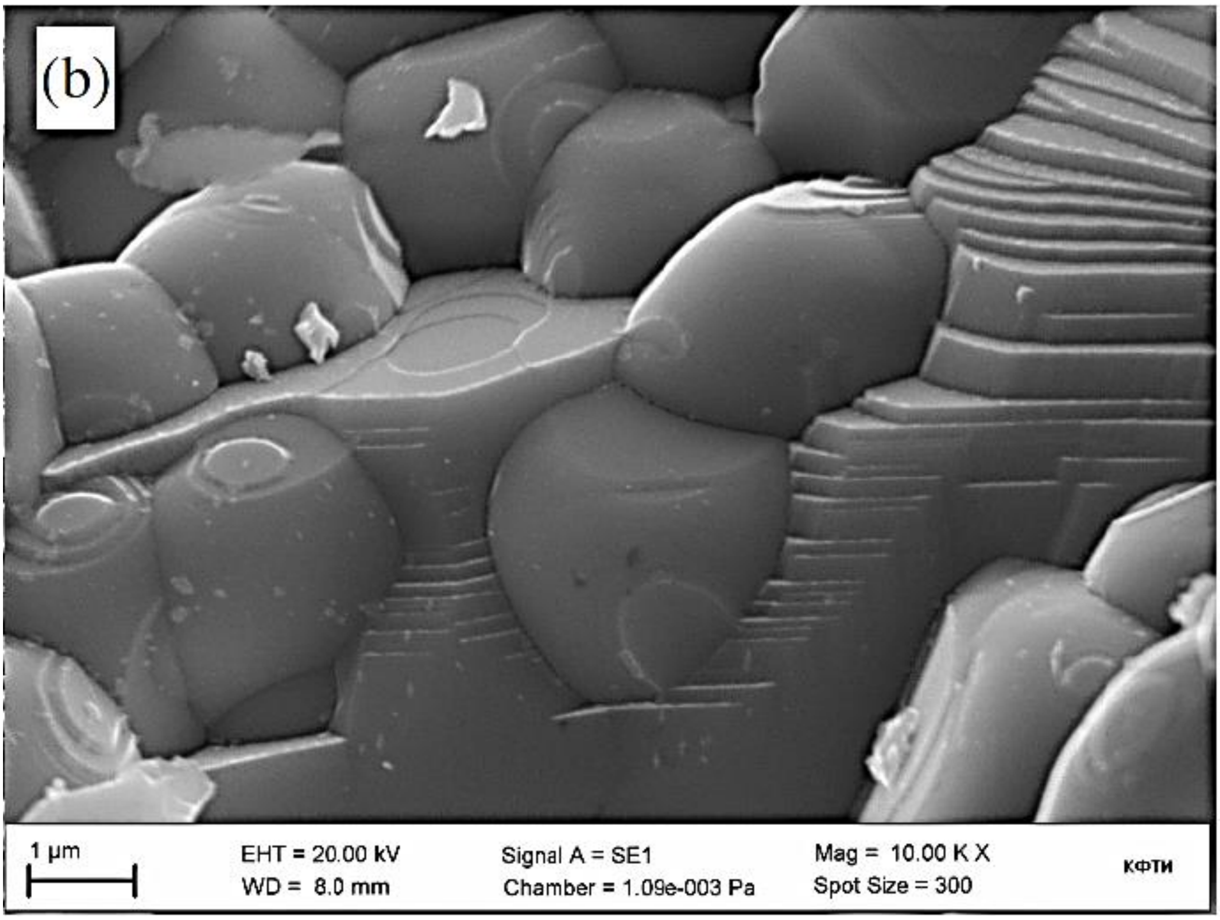

Figure 2. Surface structure of the $La_{0.5}Ba_{0.5}MnO_3$ compound on a scale of D = 1 µm.

Conclusions:

The compound $La_{0.5}Ba_{0.5}MnO_3$ was obtained, its crystal structure and morphology were studied. The study used X-ray diffraction and electron microscopy. It has been established that the structural elements of this crystal consist of MnO_6 octahedra. During cation-cation substitution, the metals La and Ba alternate at the sites of the crystal lattice. The crystal structure is formed by covalent bonds formed by metal atoms with oxygen atoms, and this structure is highly symmetrical. The morphology of the resulting sample was also studied. It was found that this compound has a densely formed shape. There are no voids between the crystallites. Crystallites are in the range D = 1-3 µm.

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