RESEARCH ARTICLE

SYNTHESIS AND X-RAY ANALYSIS OF COMPLEX FERRITE BILIFE$_2$O$_5$

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Abstract

The paper describes the synthesis and X-ray study of a complex structure of ferrite BiLiFe$_2$O$_5$. Ferrite with mixed complex oxide BiLiFe$_2$O$_5$ was synthesized by high temperature solid state reaction. The structure of the ferrites, type of syngony, parameters of the unit cells, radiographic and pycnometric densities were determined by X-ray phase analysis for the first time: $a=5.277$, $c=13.86\,\AA$, $V_{\text{unit cell}} = 1054.6\,\AA^3$, $Z=12$, $\rho_{\text{rad}} = 7.7022$, $g/\text{cm}^3$, $\rho_{\text{picn}} = 7.7031\,\text{g/cm}^3$. A comparative analysis of the relationship between crystal lattice parameters with parameters of the initial oxides and complex ferrites has been performed.

Introduction:

Semiconductor materials, which functionality is stipulated by electron charge are generally used in modern electronics. Increasing requirements to electronic devices expose the problem of search and implementation of alternative materials, working on non-classical principles. The basis of future electronic can become spintronics devices that use both electron charge and its spin [1].

Spintronics became known after opening the effect of discovery of “giant” magnetoresistance (GMR), which is stipulated by different scattering on ferromagnetic impurities of two groups of electrons’ spins with “up” and “down”. This selection requires the significant difference between the average lengths of free path of the electrons with “up” and “down” directions of the spins. This occurs in ferromagnetic materials characterizing by differences in the density of the free states of electrons caused by exchange splitting of 3d zone. This principle lays in the basis of magnetoresistive devices implementing the effects of the giant and tunnel magnetoresistance [2].

Literature data analysis shows that ortoferrites BiFeO$_3$ or so-called multiferroics are the most studied of ferrites that simultaneously have the electric polarization and magnetic ordering. The ortoferrites are prospective for implementation as the working environment in the data storage and processing devices. At the present time, the search of new materials with ferroelectric properties and specific electronic and magnetic structures is performed using the most famous multiferroic for. Substituted perovskites based on the bismuth ferrites often combine ferroelectric and weak ferromagnetic properties with the dominant antiferromagnetic ordering [2, 3].

This study is to investigate the conditions for obtaining and X-ray features of new classes of complex mixed bismuth ferrites, in which Bi$^3+$ is partially substituted by the ions of rare-earth elements and sodium.

Experimental part:

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New polycrystalline complex of bismuth ferrites were synthesized by ceramic processing technology. Bismuth oxide (III) (mark “chemically pure”), lithium carbonate (mark “highly-pure”) and iron oxide (III) (mark “chemically pure”) were used as the initial components. Solid-phase synthesis was carried using the thermal data of the initial components taking into account Tamman conditions for ceramic reactions [4,5]. Stoichiometrically calculated mixtures of initial components preliminary annealed in a muffle furnace at 400ºC for one hour, were thoroughly stirred and the calculated mixture of the starting components are thoroughly mixed and ground in an agate mortar, placed in an alundum crucibles, and annealed in a silite furnace. Annealing was performed by two stages: first stage at 600ºC for 48 h and second stage at 800ºC for 20 h [6].

Formation of new phases was controlled by X-ray scattering analysis performed using the radiologic diffractometer X-ray MiniFlex 600 (Rigaku). The conditions of analysis included: CuKα – radiation, Ni – filter, U=40 kV, I=10 mA, rotation rate – 1000 impulses/s, and time constant τ =5 s, 2θ = 10° – 90°. Diffraction peaks were evaluated using hundredpoint scale. Radiographs of the synthesized polycrystalline powders were indexed by the homology method (homologue is distorted structure type of perovskite) [7]. Pycnometric density of manganites was determined by the method described in [8]. Toluene served as indifferent liquid. The density of each ferrite was measured 4 – 5 times and the data were averaged. Table below shows the results of indexing of radiographs of ferrites.

Table 1: Indexing of radiographs of the synthesized phase composition BiLiFe₂O₅

| №  | [°2θ.] | d[Å]  | Int. [%] | Int. [%] | 10 /d срп. | hkl | 10 /d реоп. |
|----|--------|-------|----------|----------|-------------|-----|-------------|
| 1  | 12.29  | 7.198 | 0.1      | 193      | (1,1,0)     | 197 |
| 2  | 17.41  | 5.089 | 1.2      | 386      | (2,0,0)     | 384 |
| 3  | 21.37  | 4.156 | 2.6      | 578      | (2,1,1)     | 579 |
| 4  | 24.72  | 3.599 | 18.1     | 772      | (2,2,0)     | 777 |
| 5  | 27.69  | 3.219 | 100.0    | 965      | (3,1,0)     | 963 |
| 6  | 30.40  | 2.938 | 24.3     | 1158     | (2,2,2)     | 1156|
| 7  | 32.90  | 2.720 | 67.9     | 1351     | (3,3,0)     | 1355|
| 8  | 35.24  | 2.545 | 3.1      | 1543     | (3,3,2)     | 1547|
| 9  | 37.45  | 2.399 | 5.7      | 1737     | (4,0,0)     | 1735|
| 10 | 39.56  | 2.276 | 6.9      | 1930     | (0,2,4)     | 1935|
| 11 | 41.58  | 2.170 | 10.4     | 2123     | (3,3,2)     | 2121|
| 12 | 43.52  | 2.078 | 10.5     | 2315     | (4,2,2)     | 2318|
| 13 | 45.40  | 1.996 | 13.7     | 2510     | (1,3,4)     | 2515|
| 14 | 48.97  | 1.858 | 5.2      | 2896     | (5,2,1)     | 2893|
| 15 | 50.69  | 1.799 | 0.2      | 3089     | (4,4,0)     | 3086|
| 16 | 52.37  | 1.746 | 31.4     | 3280     | (0,3,5)     | 3284|
| 17 | 54.01  | 1.696 | 15.4     | 3476     | (6,0,0)     | 3474|
| 18 | 55.61  | 1.651 | 23.1     | 3668     | (5,3,2)     | 3669|
| 19 | 57.19  | 1.609 | 0.4      | 3862     | (6,2,0)     | 3867|
| 20 | 58.74  | 1.571 | 2.3      | 4051     | (5,4,1)     | 4055|
| 21 | 60.26  | 1.535 | 2.2      | 4244     | (6,2,2)     | 4242|
| 22 | 61.76  | 1.501 | 15.3     | 4438     | (6,3,1)     | 4436|
| 23 | 63.24  | 1.469 | 1.4      | 4634     | (4,4,4)     | 4638|
| 24 | 64.70  | 1.440 | 6.8      | 4822     | (3,4,5)     | 4825|
| 25 | 66.15  | 1.412 | 1.7      | 5015     | (0,4,6)     | 5017|
| 26 | 67.57  | 1.385 | 3.5      | 5213     | (7,2,1)     | 5211|
| 27 | 68.99  | 1.360 | 1.5      | 5406     | (2,4,6)     | 5408|
| 28 | 70.39  | 1.337 | 1.1      | 5594     | (0,3,7)     | 5592|
| 29 | 73.15  | 1.293 | 3.2      | 5981     | (6,5,1)     | 5981|
| 30 | 74.52  | 1.272 | 0.3      | 6180     | (8,0,0)     | 6184|
| 31 | 75.87  | 1.253 | 2.0      | 6369     | (1,4,7)     | 6366|
| 32 | 77.22  | 1.234 | 0.8      | 6567     | (0,2,8)     | 6567|
| 33 | 78.57  | 1.217 | 9.4      | 6751     | (3,5,6)     | 6755|
| 34 | 79.90  | 1.200 | 8.6      | 6944     | (6,6,0)     | 6946|
Results:
On the basis of X-ray diffraction of the synthesized compounds indexing BiLiFe$_2$O$_5$ found that ferrite crystallized in the tetragonal structure with the following unit cell parameters: $a = 5.277$, $c = 13.86\AA$, $V_{\text{unit cell}} = 1054.6\, \text{Å}^3$, $Z = 12$, $\rho_{\text{rad}} = 7.7022$, $\text{g/cm}^3$, $\rho_{\text{picn}} = 7.7031\, \text{g/cm}^3$.

The correctness of the results of the ferrite indexing confirmed the good agreement of the experimental and calculated values of the reciprocals of the squares of the distances between planes ($10^4/d^2$), consistency of values of X-ray and pycnometric densities.

Conclusions:
BiLiFe$_2$O$_5$ crystallizes in the tetragonal system, analysis of the relationship between the parameters of the crystal lattice parameters of the original $\delta$-Bi$_2$O$_3$ shows equality and parameter and increase the value of the parameter to twice the sum of the values of the even squares Miller index ($h^2 + k^2 + l^2$) shows a body nature of the crystal lattice.

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