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ИССЛЕДОВАНИЕ МИНЕРАЛОГИЧЕСКОГО СОСТАВА, СТРУКТУРЫ И СВОЙСТВ ПОВЕРХНОСТИ ЗОЛЬНЫХ МИКРОСФЕР УКРАИНЫ

Исследованы свойства (минералогический состав, смачиваемость, пористость, удельная поверхность и ее энергетическое состояние) зольных микросфер различных ТЭС Украины, получаемых в результате сжигания угля Донецкого (Трипольская, Кураховская, Криворожская и Приднепровская ТЭС) и Львовско-Волынского угольных бассейнов (Бурштынская ТЭС). Проанализировано влияние свойств поверхности зольных микросфер на их потенциальную способность использования в качестве наполнителей для строительных материалов.

Ключевые слова: зольные микросферы, удельная поверхность, минералогический состав, порошкообразный материал, аморфная фаза.

Demchenko Valentyna, *Postgraduate Student, Department of Commodity and Customs Affairs, Kyiv National University of Trade and Economics, Ukraine, e-mail: tina76748@gmail.com, ORCID: http://orcid.org/0000-0001-7527-2236*

Simyachko Olena, *PhD, Associate Professor, Department of Commodity and Customs Affairs, Kyiv National University of Trade and Economics, Ukraine, e-mail: olesim@ukr.net, ORCID: http://orcid.org/0000-0002-5229-8000*

Svidersky Valentin, *Doctor of Technical Sciences, Professor, Head of the Department of Chemical Technology of Composite Materials, National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute», Ukraine, e-mail: xtkm@kpi.ua, ORCID: http://orcid.org/0000-0002-2246-3896*

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Zavodyannyy V.

CRYSTALLINE STRUCTURE ANALYSIS OF Ba_3WO_6 COMPOUND

Показано, що сполука Ba_3WO_6 має три поліморфні модифікації, дифракційні спектри яких розміщенні в базах даних pdf-2 за 2004 р. За спектром згенерованим HiphScorePlus 3.0 під номером 00-033-0182 сполука належить до структури типу $Ba_{11}W_4O_{23}$. Уточнено періоди решітки, мікроструктурні параметри та стехіометричний склад сполуки Ba_3WO_6.

Ключові слова: *рентгеноструктурний аналіз, база даних pdf-2, Ba84.46W31.07O189.08, метод Рітвельда.*

1. Introduction

Metal-porous cathodes are widely used in electric rocket engines of space vehicles, as well as in powerful electric vacuum devices, for example, microwave range. They combine a large number of composite cathodes and are multiphase systems consisting of a metal matrix (sponge), in the pores and on the surface of which an emission-active substance is located. In the process of impregnating the sponge with an emission active substance, Ba_3WO_6 is formed, which explains the presence of barium on the emitter surface [1]. Consequently, studies of the properties of this compound, in particular its crystal structure, are relevant.

2. The object of research and its technological audit

The object of research is Ba_3WO_6 crystal structure. This compound is formed from a mixture of $BaCO_3$ i WO_3, which is heated at 1000–1400 °C for 30 hours, followed by hardening. At 690 °C, polymorphic transformation of Ba_3WO_6 from triclinic crystal system to cubic is observed. Also, this compound can be synthesized from a mixture of oxides at a pressure of 7 kbar, a temperature of 1300 °C and a holding time of 24 hours [2].

One of the most problematic places is the presence of a large number of diffraction spectra captured for this compound, obtained by the Bragg-Bertrand method on copper filtered radiation.

For example, in the pdf-2 database for 2004, there are 7 diffraction spectra of different quality are obtained for the Ba_3WO_6 compound synthesized by various methods.

3. The aim and objectives of research

The aim of this work is studying the crystal structure of Ba_3WO_6 compound, presented in the diffraction data base pdf-2 for 2004 at the number 00-033-0182.

For the set aim the following tasks are solved:

1. To conduct X-ray phase analysis for the presence of compounds indicated in the state diagram (Fig. 1).

2. Taking into account the results of the phase analysis, to propose a model of the microstructure parameters of the spectrum of this compound.

3. To refine the microstructural parameters of this compound by the Rietveld method.

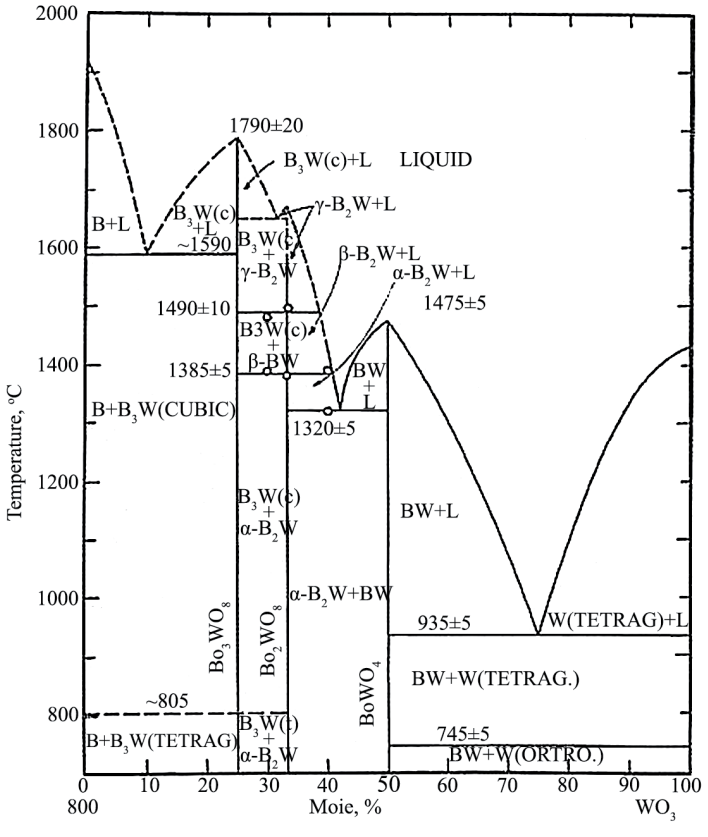

Fig. 1. The phase diagram of BaO-WO_3 according to [3]: L – liquidus line; C and CUBIC – cubic crystal structure; TETRAG – tetragonal crystal structure; ORTHO – orthorhombic crystal structure; B – BaO; W – WO_3; Ba_3W – Ba_3WO_6

4. Research of existing solutions of the problem

Data of pdf-2 for 2004 [4] indicate the presence of seven Ba_3WO_6 diffraction spectra of Ba_3WO_6 (Table 1). Positions 5, 6 and 7 are interest (Table 1).

Table 1

Information on the Ba_3WO_6crystal structure

No.	Compound	Crystal structure	Lattice periods, A°	Card number in the pdf-2 database	Diffraction spectrum quality
1	Ba_3WO_6	Unknown	Unknown	00-015-0240	Low quality
2	Ba_3WO_6	Unknown	Unknown	00-020-0152	Low spectrum accuracy
3	Ba_3WO_6	Tetragonal	a = 8.6520 b = 8.6520 c = 16.4340	00-025-0082	Doubtful quality
4	Ba_3WO_6	Orthorhombic	a = 12.1800 b = 12.2300 c = 17.3700	00-026-0195	Indexed
5	Ba_3WO_6	Cubic, Fm-3m	a = 17.1765 b = 17.1765 c = 17.1765	00-033-0182	The highest quality of the diffraction spectrum
6	Ba_3WO_6	Triclinic, P1	a = 6.1072 b = 6.1071 c = 8.6710 α = 90.0200° β = 89.9800° γ = 90.0400°	01-077-0642	The calculated spectrum by the structural model
7	Ba_3WO_6	Cubic, Fm-3m	a = 8.62 b = 8.62 c = 8.62	01-089-5178	The calculated spectrum by the structural model

According to [5], the crystal structure of the spectrum, represented in position 6 of Table 1, has the following microstructural parameters: triclinic, crystal structure P1, lattice parameters a=6.1072 A°; b=6.1071 A°; c=8.6710 A°; α=90.0200°; β=89.9800°; γ=90.0400°; Z=2. The microstructural parameters are presented in Table 2.

Table 2

The microstructural parameters of Ba_3WO_6 according to [5]

Atom	The correct point system	x	y	z	The filling factor of the positions
Ba(1)	1a	0.0	0.0	0.0	1.0
Ba(2)	1a	0.528	0.44	0.516	1.0
Ba(3)	1a	0.01	0.96	0.487	1.0
Ba(4)	1a	0.505	0.481	0.028	1.0
Ba(5)	1a	0.031	0.414	0.729	0.5
Ba(6)	1a	0.052	0.546	0.758	0.5
Ba(7)	1a	0.54	0.012	0.25	0.5
Ba(8)	1a	0.558	0.909	0.276	0.5
W(1)	1a	–0.001	0.465	0.25	1.0
W(2)	1a	0.484	0.966	0.767	1.0
O(1)	1a	0.768	0.673	0.272	1.0
O(2)	1a	0.991	0.461	0.031	1.0
O(3)	1a	0.795	0.262	0.325	1.0
O(4)	1a	0.982	0.398	0.467	1.0
O(5)	1a	0.236	0.259	0.255	1.0
O(6)	1a	0.23	0.66	0.296	1.0
O(7)	1a	0.314	0.228	0.768	1.0
O(8)	1a	0.277	0.737	0.76	1.0
O(9)	1a	0.488	0.96	0.989	1.0
O(10)	1a	0.503	0.926	0.552	1.0
O(11)	1a	0.706	0.752	0.78	1.0
O(12)	1a	0.708	0.187	0.762	1.0

In [6], for the spectrum presented in position 7 (Table 1), the crystal structure is represented by the following data: the compound has a cubic crystal structure, Fm-3m and a lattice period a=8.62 A°. Microstructural parameters are given in Table 3.

Table 3

The microstructural parameters of Ba_3WO_6 according to [6]

Atom	The correct point system	x	y	z	The filling factor of the positions
Ba(1)	8c	0.25	0.25	0.25	1.0
Ba(2)	4b	0.5	0.5	0.5	1.0
W	4a	0	0	0	1.0
O	24e	0.2	0	0	1.0

The phase diagram of BaO-WO_3 is shown in Fig. 1 according to [3], where Ba_3WO_6 is indicated. There are several polymorphic modifications: cubic, tetragonal, partially confirmed by pdf-2 data for 2004 [4].

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It is noted in [7] that the obtained Ba_3WO_6 barium tungstate compound has a cryolite structure that is rhombically distorted. This compound is indexed under the assumption that it belongs to a rhombic system with lattice periods a=12.18 A°, b=12.23 A°, c=17.37 A°, the diffraction spectrum of which is contained in pdf-2 to 2004 under number 00-026-0195.

An isothermal cross section of the phase diagram of the Ba-W-O system at a temperature of 1700 °C is given in [8] (Fig. 2). As can be seen from the phase diagram of the compound Ba_3WO_6+W is on the line of double compounds BaO and WO_3. At the same time, there is a large triple region in which the input chemical elements exist in the liquid state. This may indicate that the Ba_3WO_6 compound may have a significant homogeneity region.

The existence of compounds based on Ba_3WO_6, such as: $Sr_{3-x}Ba_xWO_6$ (x=0–0.75) Ba3-xWO6: xEu3+(x=0.01, 0.03, 0.05, 0.08, 0.1), is noted in [9, 10] have a crystalline structure of the (NH_4) $3FeF_6$ (cubic crystal structure), which agrees well with the data of [6]. In particular, the synthesized compounds have ferroelectric and luminescent properties, which can be used, for example, in solid-state lighting devices.

Special attention should be paid to the works [11, 12], where it is synthesized at 1300 °C and quenched with liquid nitrogen, and the crystal structure of the new compound $Ba_{11}W_4O_{23}$ is investigated, which has its own structural type. The structure of $Ba_{11}W_4O_{23}$ is investigated by X-ray and neutron diffraction analysis, using the Rietveld method (Fd-3m, a=17.1823 (1) Å, Z=8, Rp=3.09 %, Rwp=4.25 %). The structure is an example of a superstructure of a simple perovskite ABO3, and it can be written as Ba1.75–0.25) BaWO5.75–0.25, that has vacancies on both the metal and the anion. The local structure of one of the two asymmetric tungsten ions is the WO_6 octahedron, which is characteristic of perovskite. Another tungsten, surrounded by oxygen and anion vacancies, statistically distributed over three separated sections, with the formation of 18 partially occupied oxygen atoms (on average ~30 %), represented as WO (18/3), between adjacent WO18/3 polyhedra. that $Ba_{11}W_4O_{23}$ at room temperature is isostructural to the high-temperature phase at 1100 °C.

So $Ba_{11}W_4O_{23}$ (or Ba1.75 (BaW) O5.75) has a derivative of the perovskite structure (ABO3) with vacancies located in the A sub-lattice, but disordered in the O sub-lattice, which indicates the potential as the electrolyte of the oxide ion.

The spectrum of the compound of position 5 deserves special attention (Table 1). According to the data of [5], the spectrum of the compound is indexed in cubic crystal structure, Fm-3m, lattice constant a=17.1765 A°. At the same time, the literature data [11–13] indicate that this compound belongs to the new structural type $Ba_{11}W_4O_{23}$. The microstructural parameters are given in Table 4, the lattice periods are 17.188 (5) A°, Fd-3m (the second subgroup).

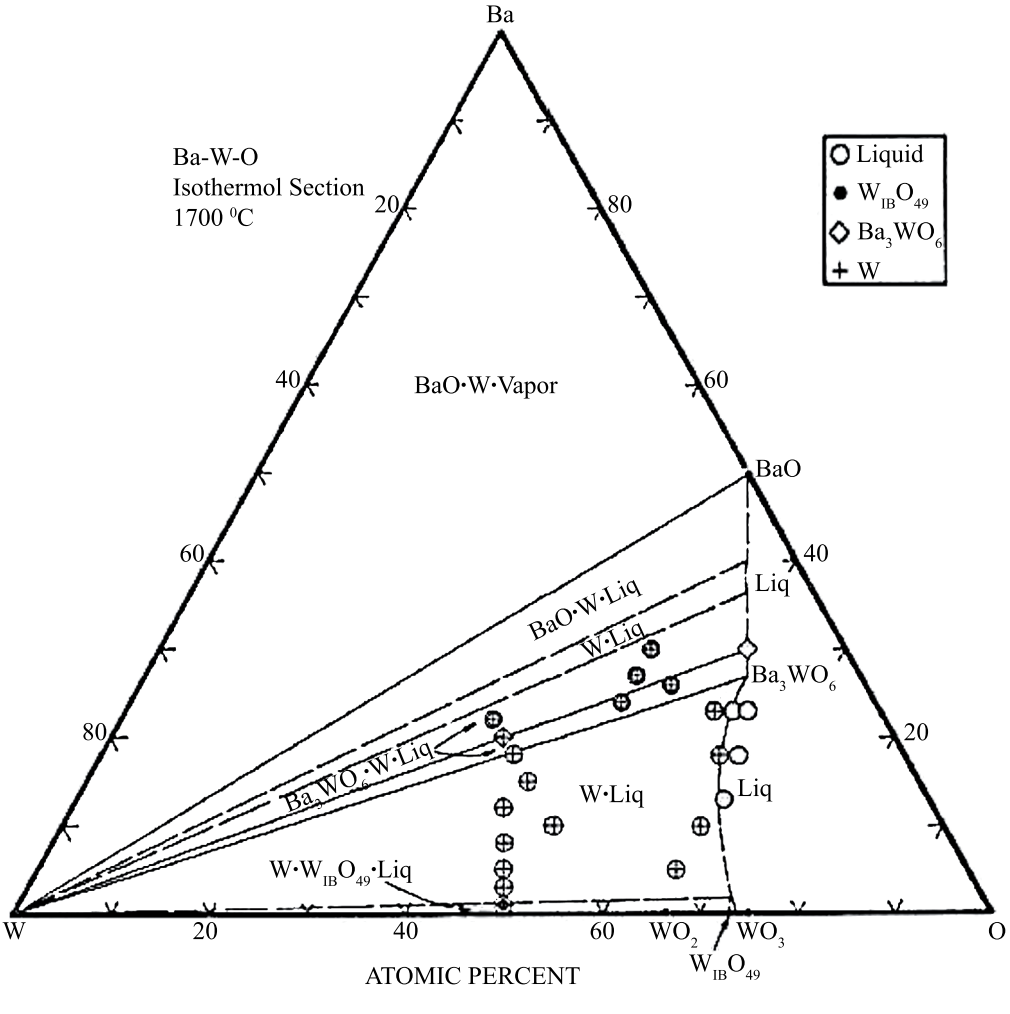

Fig. 2. Isothermal section of the phase diagram of the Ba-W-O system at a temperature of 1700 °C

Table 4

Microstructural parameters of $Ba_{11}W_4O_{23}$

Atom	The correct point system	*x*	*y*	*z*	The filling factor of the positions	U_{iso} [a]
Ba1	8b	0.375	0.375	0.375	1	2.1(2)
Ba2	48f	0.4002(1)	0.125	0.125	1	3.3(1)
Ba3	32e	0.22556(8)	0.22556(8)	0.22556(8)	1	5.1(1)
W1	16d	0.5	0.5	0.5	1	1.3(1)
W2	16c	0	0	0	1	2.2(1)
O1	96g	0.49970(7)	0.49970(7)	0.61246(7)	1	2.4(1)
O2	96g	0.0779(2)	0.0779(2)	–0.0064(3)	0.412(1)	6.2(4)
O3	96h	0.0762(2)	–0.0762(2)	0	0.308(1)	9.0(9)
O4	96g	0.1037(5)	–0.0063(4)	–0.0063(4)	0.197(1)	9.7(8)

The described studies aimed to refine the microstructural parameters for joining position 5 (Table 4).

5. Methods of research

The diffraction spectrum for the study is generated using the HiphScorePlus 3.0 program and the attached pdf-2 database for 2004 in the UDF format.

X-ray phase analysis is performed using the HiphScorePlus 3.0 program. Microstructures parameters of known compounds are found with the help of [4, 14, 15].

An analysis of the proposed structural model of this spectrum is also carried out using the HiphScorePlus 3.0 program by the Rietveld method.

6. Research results

X-ray diffraction analysis indicates the absence of additional phases. Thus, the investigated spectrum is single-phase. A refinement of the crystal structure of this compound is carried out using the HiphScorePlus 3.0 program by the Rietveld method. The compound belongs to the cubic structure Fd-3m (the second subgroup) with a lattice period a=17.1690 (4) A°. The microstructural parameters of the phase are given in Table 5.

The values of the interplanar distances and intensities, observed and calculated from this model, are given in Table 6.

Table 5

Microstructural parameters of Ba_3WO_6 compound

Atom	The correct point system	The filling factor of the positions	x	*y*	*z*	Temperature factor
Ba1	8b	0.894304	0.375000	0.375000	0.375000	0.500000
Ba2	48f	0.943957	0.400354	0.125000	0.125000	2.296785
Ba3	32e	1.000000	0.222107	0.222107	0.222107	0.549590
W1	16d	1.000000	0.500000	0.500000	0.500000	0.500000
W2	16c	0.941749	0.000000	0.000000	0.000000	0.500000
O1	96g	1.000000	0.504385	0.504385	0.615905	0.000000
O2	96g	0.552858	0.044073	0.044073	–0.036847	0.500000
O3	96h	0.215246	0.094419	–0.094419	0.000000	0.000000
O4	96g	0.201508	0.108406	0.108406	–0.074564	5.500592

Table 6

The values of interplanar distances and observed and calculated intensities

d_{cal}(A°)	d_{obs}(A°)	I_{cal}	I_{obs}	*H*	*K*	*L*
9.92545	9.88879	1.28	1.98	1	1	1
6.07498	6.07453	0.81	1.98	0	2	2
5.18014	–	0.15	–	1	1	3
4.95946	4.96180	9.12	8.96	2	2	2
4.29464	4.29579	5.68	4.99	0	0	4
3.94085	3.94189	1.88	2.98	1	3	3
3.50619	3.50904	4.24	4.95	2	2	4
3.30558	3.30703	5.77	24.96	1	1	5
3.30558	–	19.22	–	3	3	3
3.03626	3.03602	100.00	100.00	0	4	4
2.90316	2.90497	0.05	0.94	1	3	5
2.86254	2.86302	3.25	2.96	2	4	4
2.71559	2.71595	1.27	0.94	0	2	6
2.61911	2.62005	1.73	2.00	3	3	5
2.58917	2.59006	7.85	7.96	2	2	6
2.47890	–	0.04	–	4	4	4
2.40486	2.40503	0.01	2.99	1	1	7
2.40486	–	3.17	–	1	5	5
2.29496	–	0.42	–	2	4	6
2.23583	2.23601	4.85	13.95	1	3	7
2.23583	–	8.00	–	3	5	5
2.14669	2.14601	15.71	16.87	0	0	8
2.09807	–	0.43	–	3	3	7
2.08258	2.08397	0.24	0.90	4	4	6
2.02389	2.02401	2.11	2.91	0	6	6
2.02389	–	1.32	–	2	2	8
1.98298	1.98410	5.33	4.90	1	5	7
1.98298	–	0.11	–	5	5	5
1.96989	1.96939	5.33	4.93	2	6	6
1.92000	1.92060	0.64	3.96	0	4	8
1.88497	–	0.34	–	1	1	9
1.88497	–	0.03	–	3	5	7
1.87371	1.87369	3.62	1.95	2	4	8
1.83062	1.83079	0.79	0.94	4	6	6
1.80019	1.80050	3.38	3.95	1	3	9
1.75267	1.75220	18.84	20.96	4	4	8
1.72590	1.72619	0.30	0.94	1	7	7
1.72590	–	1.04	–	3	3	9
1.72590	–	0.01	–	5	5	7
1.68389	1.68400	0.97	1.93	0	2	10
1.68389	–	1.30	–	2	6	8
1.66011	1.66021	3.01	8.96	1	5	9
1.66011	–	5.59	–	3	7	7
1.65241	1.65219	1.21	5.99	2	2	10
1.65241	–	6.25	–	6	6	6
1.60131	–	1.11	–	3	5	9
1.59440	1.59354	0.45	0.62	4	6	8
1.56759	–	0.06	–	2	4	10
1.54835	1.54851	1.07	0.92	5	7	7
1.54835	–	0.00	–	1	1	11
1.51780	1.51789	6.92	6.91	0	8	8
1.50032	1.50097	0.15	0.93	1	7	9
1.50032	–	0.27	–	5	5	9
1.50032	–	0.14	–	1	3	11
1.49462	1.49514	2.13	0.91	2	8	8
1.49462	–	0.02	–	4	4	10
1.47247	–	0.00	–	0	6	10
1.47247	–	0.31	–	6	6	8
1.45649	1.45672	0.72	3.11	3	3	11
1.45649	–	1.04	–	3	7	9
1.45128	1.45159	7.23	7.04	2	6	10
1.43098	1.43130	0.01	1.94	0	0	12
1.43098	–	0.82	–	4	8	8
1.41630	1.41658	0.00	0.90	1	5	11
1.41630	–	1.46	–	7	7	7
1.39280	1.39340	0.55	2.99	2	2	12
1.39280	–	3.01	–	4	6	10
1.37926	1.37970	0.01	0.95	3	5	11
1.37926	–	0.09	–	5	7	9
1.35753	–	3.37	–	0	4	12
1.34498	1.34570	0.85	6.99	1	9	9
1.34087	–	0.38	–	2	4	12
1.34087	–	0.83	–	6	8	8

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Table 7 shows the interatomic distances of the Ba_3WO_6 compound under the number 00-015-0240 in the pdf-2 database for 2004.

And Fig. 3 shows the resultant diffractograms, generated and calculated from the microstructure parameters of the $Ba_{84.46}W_{31.07}O_{189.08}$ compound.

The performed studies of the crystal structure of the compound (Fig. 4) indicate that the test compound is obtained from $BaCO_3$ and WO_3 (ratio 73:27 mol).

The compound is heated in Au (gold) crucible in air at 950 °C for 48 hours. This sample is approximately 2 ml. % richer on WO_3 than the true 3:1 oxide and has a stoichiometric composition shifted.

This assumption is confirmed by the clarification of the crystal structure of the compound obtained from pdf-2 for 2004 [4] and it is $Ba_{84.46}W_{31.07}O_{189.08}$.

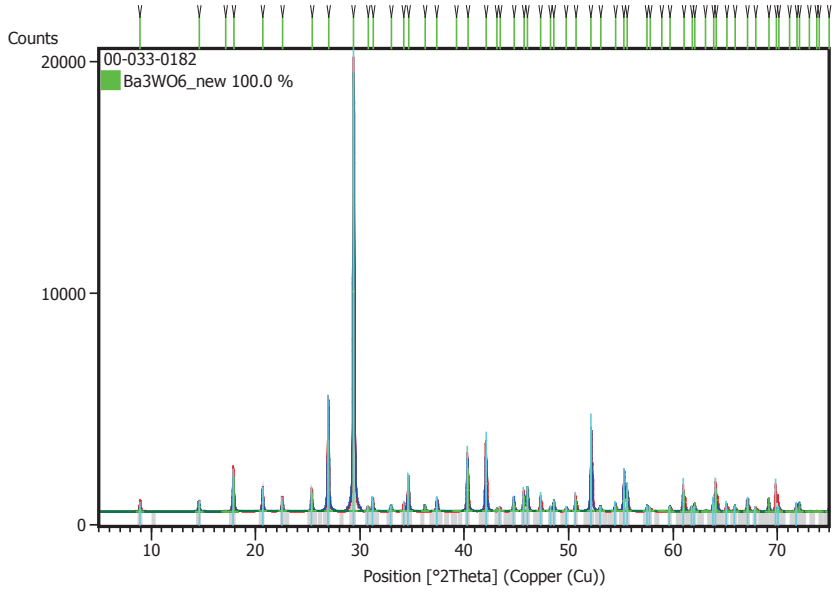

Fig. 3. The resultant diffractograms, generated and calculated from the microstructure parameters of the $Ba_{84.46}W_{31.07}O_{189.08}$ compound

Table 7

The interatomic distances of the test compound

Atom1	Atom2	Distance, A°	Atom1	Atom2	Distance, A°
Ba1	–O	2.933	O3	–W	1.243
Ba2	–O	1.362	–	–O	1.516
–	–O	2.409	–	–O	1.691
–	–O	2.739	–	–O	1.965
–	–O	2.767	–	–O	2.455
–	–O	3.154	–	–O	2.486
–	–W	3.484	–	–O	2.608
Ba3	–O	2.890	–	–Ba	2.767
–	–O	2.969	–	–O	2.939
–	–O	3.073	–	–Ba	3.264
–	–O	3.264	–	–O	3.362
W1	–O	1.993	–	–O	3.404
–	–Ba	3.484	O4	–O	1.516
W2	–O	1.243	–	–O	1.907
–	–O	2.293	–	–W	2.293
–	–O	2.927	–	–O	2.293
O1	–W	1.993	–	–Ba	2.409
–	–O	2.708	–	–O	2.585
–	–Ba	2.739	–	–O	2.608
–	–O	2.831	–	–O	2.831
–	–Ba	2.890	–	–Ba	3.073
–	–O	2.925	–	–O	3.362
–	–Ba	2.933	–	–	–
–	–O	3.149	–	–	–
–	–Ba	3.154	–	–	–
O2	–W	1.993	–	–	–
–	–O	2.708	–	–	–
–	–Ba	2.739	–	–	–
–	–O	2.831	–	–	–
–	–Ba	2.890	–	–	–
–	–O	2.925	–	–	–
–	–Ba	2.933	–	–	–
–	–O	3.149	–	–	–
–	–Ba	3.154	–	–	–
–	–O	3.328	–	–	–

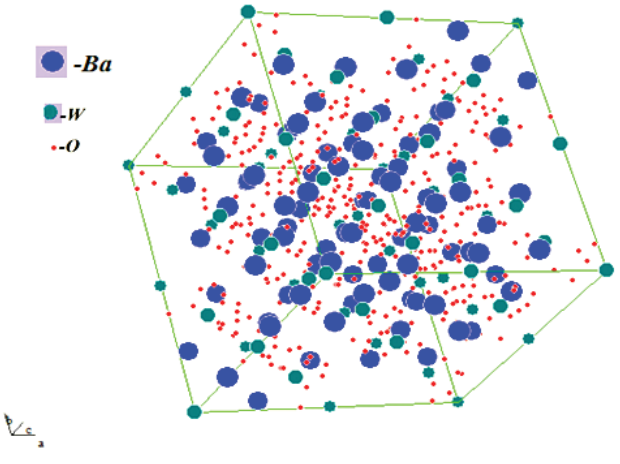

Fig. 4. Images of the crystal structure of $Ba_{84.46}W_{31.07}O_{189.08}$ compound

7. SWOT analysis of research results

Strengths. As a result of the study, it is established that Ba1, Ba2 atoms have vacancies in regular systems of points 8b, 48f. Also, the result of reducing the filling of positions for the tungsten atom W2 (16c) is obtained. The oxygen atoms, in contrast to the input model, also have incomplete filling of the correct points systems (O2, O3, O4). In addition, the calculation shows that the coordinates of the atoms O2 (96g) and O3 (96h) differ from the input model in proportion to 2 and 1.5 times.

Weaknesses. Incomplete filling of correct points systems by atoms is associated with a change in the stoichiometric composition of the compound. A significant relative change in the coordinates of the oxygen atoms leads to a distortion in the O-sub-lattice of the perovskite structure with vacancies (ABO3).

Opportunities. A polymorphic transformation from triclinic crystal structure into cubic is recorded without changing the stoichiometric composition of the compound at a temperature of 690 °C. At the same time, there are data on this compound relating to orthorhombic and tetragonal crystal

structure, and possibly depends on the method of obtaining the compound. Also displaced stoichiometric composition of $Ba_{11}W_4O_{23}$ indicates the presence of a homogeneity region of this compound, the boundaries of which are worth exploring. The formation of this compound can be affected by the method of its preparation and impurities, which can somewhat change the structural parameters.

Threats. The compounds $Ba_{11}W_4O_{23}$ and Ba_3WO_6 are close to each other in their stoichiometric composition, but they differ in crystalline structures, and the first of them has a homogeneity region. Obviously, they also have different physicochemical properties. Perhaps the formation of these compounds is affected not so much by the percentage of incoming materials, but by the method of obtaining the compounds themselves. Therefore, in the synthesis of these compounds it is necessary to take into account this.

8. Conclusions

1. The conducted X-ray phase analysis doesn't reveal the presence of several phases in the investigated compound, presented in the state diagram (Fig. 1, Table 1). So it is concluded that the compound is single-phase.

2. Using the HiphScorePlus 3.0 program, the Riffveld method is used to study the diffraction spectrum of the compound under the number 00-033-0182. It is revealed that the input model is $Ba_{11}W_4O_{23}$ structural type [11–13].

3. It is found that the compound belongs to the cubic system, the spatial symmetry group Fd-3m, has a constant crystal lattice of 17.1690 (4) A° (Table 4). The disagreement factor is $R=5.43404$. The displaced stoichiometric composition can mean that this compound has a significant area of homogeneity, the boundaries of which can be the subject of further research.

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АНАЛИЗ КРИСТАЛЛИЧЕСКОЙ СТРУКТУРЫ СОЕДИНЕНИЯ BA_3WO_6

Показано, что соединение Ba_3WO_6 имеет три полиморфные модификации, дифракционные спектры которых размещены в база данных pdf-2 за 2004 г. По спектру сгенерированным HiphScorePlus 3.0 под номером 00-033-0182 соединение входит в структуру типа $Ba_{11}W_4O_{23}$. Уточнены периоды решетки, микроструктурные параметры и стехиометрический состав соединения Ba_3WO_6.

Ключевые слова: рентгеноструктурный анализ, база данных pdf-2, $Ba_{84.46}W_{31.07}O_{189.08}$, метод Ритвельда.

Zavodyannyy Viktor, *PhD, Associate Professor, Department of Physics and General Engineering Disciplines, Kherson State Agriculture University, Ukraine, e-mail: zavodyannyy@gmail.com, ORCID: http://orcid.org/0000-0002-8224-8215*