CORRELATION BETWEEN CRYSTAL LATTICE PARAMETERS AND CRITICAL SUPERCONDUCTING PROPERTIES OF YBCO-123: A STATISTICAL STUDY

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Abstract. The article talks about production technologies of yttrium-based YBCO-123 cuprate, which is part of high-temperature superconductor (HTS) cuprates, and its critical parameters. In this, the analysis of the results obtained by the scientists of the world regarding the study of this sample and the results available to us were compared. A chronology of articles published in international scientific sources in the last 10 years on the research of Y-123 cuprate was developed. The effect of the change in the value of δ on the structure of the crystal lattice in the samples obtained based on the $YBa_2Cu_3O_{7-\delta}$ formula was expressed based on the analysis of sources. The electrophysical properties of the YBCO sample were studied.

Key words: HTS, YBCO, Solid state reaction, orthorhombic, tetragonal, crystal lattice, Miessner effect.

Annotatsiya. Ushbu maqolada yuqori haroratli o‘tao‘tkazgich (HTS) kupratlar tarkibiga kiruvchi ittriy asosidagi YBCO-123 kupratining olinishi texnologiyalari va uning kritik parametrlari yoritilgan. Bunda mazkur namuna bo‘yicha dunyo olimlari tomonidan o‘tkazilgan tadqiqotlar natijalari hamda biz tomonidan olingan natijalar qiyosiy tahlil qilingan. So‘nggi 10 yil davomida Y-123 kupratini tadqiq etishga bag‘ishlangan xalqaro ilmiy manbalarda chop etilgan maqolalar xronologiyasi shakllantirilgan. $YBa_2Cu_3O_{7-\delta}$ formulasi asosida olingan namunalarda δ qiymatining o‘zgarishi kristall panjara tuzilishiga ko‘rsatadigan ta’siri manbalar tahlili asosida ifodalangan. YBCO namunalarining elektrofizik xossalari tadqiq etilgan.

Kalit so‘zlar: YYO‘O‘, YBCO, qattiq fazali reaksiya, ortorombik, tetragonal, kristall panjara, Miessner effekti.

Аннотация. В данной статье рассматриваются технологии получения иттрийсодержащего купрата YBCO-123, относящегося к классу высокотемпературных сверхпроводящих (ВТСП) купратов, а также его критические параметры. Проведён сравнительный анализ результатов исследований, полученных ведущими учёными мира по изучению данного образца, с результатами, полученными авторами работы. Сформирована хронология статей, опубликованных за последние 10 лет в международных научных источниках, посвящённых исследованию купрата Y-123. На основе анализа литературных данных показано влияние изменения значения δ на

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структуру кристаллической решётки образцов, полученных по формуле $YBa_2Cu_3O_{7-\delta}$. Исследованы электрофизические свойства образцов YBCO.

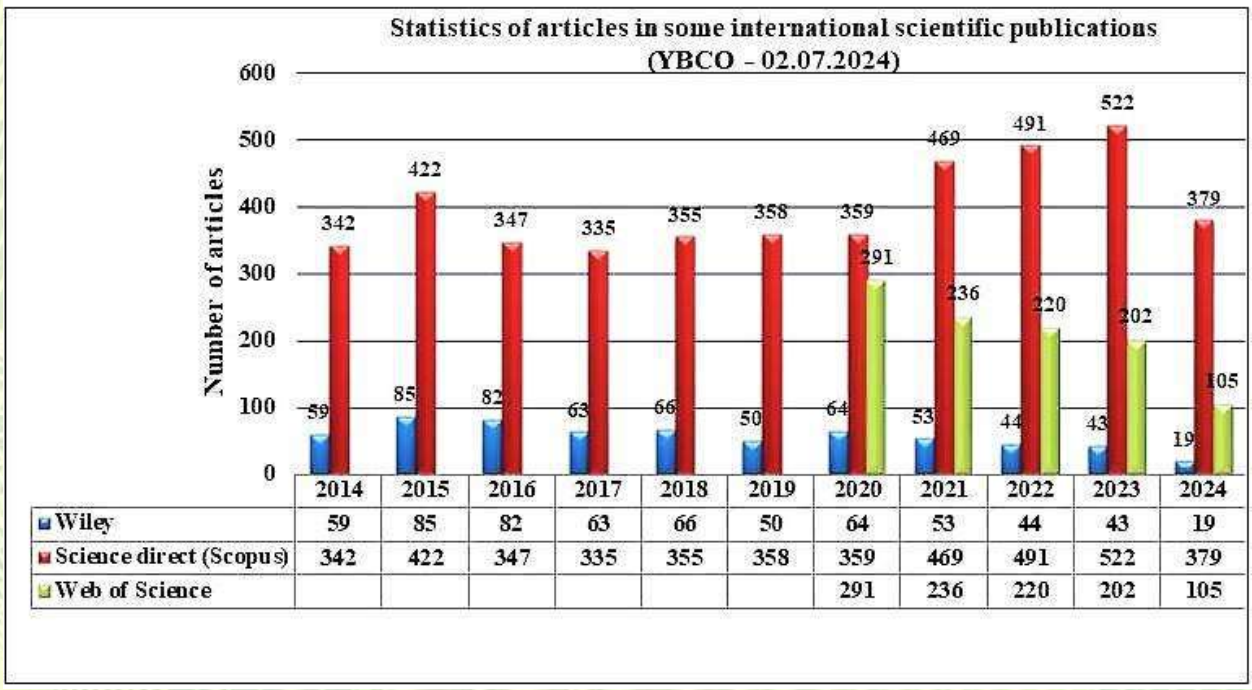
Ключевые слова: ВТСП, YBCO, твердофазная реакция, орторомбическая структура, тетрагональная структура, кристаллическая решётка, эффект Мейсснера.

1. INTRODUCTION.

Currently, high-temperature superconductors (HTS) are used in various fields, such as non-contact magnetic bearings, magnetic bearing high-speed trains (Maglev) and energy storage systems, etc. Magnetic levitation force in vertical direction In order to increase the loading capacity and stability of Maglev systems, it is necessary to increase the lateral guiding force. However, this leads to an increase in the cost of the Maglev system, as the main cost of these systems is the construction of PMGs over kilometers between cities or countries. Another way to improve the magnetic strength properties is to improve the superconducting properties of HTS. In recent years, YBCO cuprate superconductors have been used as HTS in Maglev systems due to their high critical current density and ability to hold currents.

2. Experimental methods

Before researching yttrium-based cuprates (YBCO or Y-123), the state of research of such samples by world scientists was determined through literature analysis. For this, the statistical analysis of some international scientific publications was studied (Fig. 1).



	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024
Wiley	59	85	82	63	66	50	64	53	44	43	19
Science direct (Scopus)	342	422	347	335	355	358	359	469	491	522	379
Web of Science							291	236	220	202	105

Figure 1. Last 10-year statistics of articles published in international scientific journals on YBCO cuprate research.

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This chart shows the number of publications by year of articles available in Science direct, Wiley and Web of Science scientific literature lists. According to the dynamics of change for each year, we can see that the number of articles published in journals available in the Wiley and Web of Science lists of scientific literature decreases over the years without significant changes. However, it can be seen that the number of articles published in Scopus indexed journals has only been increasing since 2017, which indicates a significant increase in the scope of work in this field. The publication of 522 articles in 2023 alone and 379 articles by the end of the II quarter of 2024 indicates that the field is gaining attention.

2.1. Methods of synthesizing YBCO cuprate

There are several ways to synthesize YBCO:

- Solid-State Reaction Method;
- Sol-Gel Method;
- Chemical Wet Method;
- Melt-Quench Method;

We chose a solid-state reaction method for the synthesis of the YBCO sample. The traditional solid-state reaction route for the synthesis of cuprates consists of grinding the corresponding metal oxides or carbonates and then mixing them by calcination at high temperature to ensure interdiffusion of cations. A chemical reaction takes place through the diffusion of ions in a solid state, characterized by a slow kinetic speed. The degree of mixing and the size of the dust particles are of particular importance. The reaction starts at the points of contact between the initial components and proceeds sequentially with ionic interdiffusion through the YBa_2 product phase. Because of the short diffusion paths, the initial reaction is fast, but the subsequent reaction is slower. In many cases, a series of unwanted steps will appear. In this way, a macromolecular crystal lattice of cuprate is formed [1].

3. Result and discussion

The calcination temperature and critical parameters for obtaining yttrium-based cuprates were studied. Arranged in the order specified in the table below.

Table 1.

Analysis of critical parameters of YBCO

№	Composition ($YBa_2Cu_3O_{7-\delta}$)	Crystal lattice parameters			V (Å^3)	δ	$Calc.t$,(°C)	Tc (K)	ΔT	Source
		a, (Å)	b, (Å)	c, (Å)						
1	$YBa_2Cu_3O_{6.92}$	3.8	3.9	11.7	173.394	0.08	920	90	3.5	[3]

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2	$YBa_2Cu_3O_{6.9}$	3.8227	3.8872	11.6802	173.563	0.1	920	91.95	5.45	[4]
3	$YBa_2Cu_3O_{6.4}$	3.82	3.89	11.67	173.414	0.6	910	90	3	[5]
4	$YBa_2Cu_3O_{6.72}$	3.831	3.8502	11.6809	172.295	0.28	850	91.68	5.48	[6]
5	$YBa_2Cu_3O_{6.71}$	3.825	3.887	11.671	173.522	0.29	950	93	11	[7]
6	$YBa_2Cu_3O_{6.84}$	3.806	3.882	11.6789	172.554	0.16	950	93.5	4.5	[8]
8	$YBa_2Cu_3O_{6.92}$	3.8224	3.8941	11.6858	173.941	0.08	940	100	12	Ours

This table shows the relation of YBCO cuprate to the critical parameters of the crystal lattice dimensions. The results obtained by world researchers in different countries were analyzed. It can be seen in the table that the critical temperature T_C of the sample increases as the value of δ decreases. According to theoretical data, it accepts values $0 \leq \delta \leq 1$. If $\delta = 0$, the crystal lattice is tetragonal, and the sample shows properties of semiconductors. If $\delta = 1$, the crystal lattice is orthorhombic, and this is the shape required for superconductivity. When d takes values close to zero, the crystal lattice volume also takes maximum values. When the volume increases, the critical temperature value also increases due to the width of the movement area for the current carriers. As a result of our research, it can be seen that the crystal lattice presented in the table was formed in the largest volume, therefore, the highest critical temperature $T_C=100\ K$ was reached.

Crystal structure

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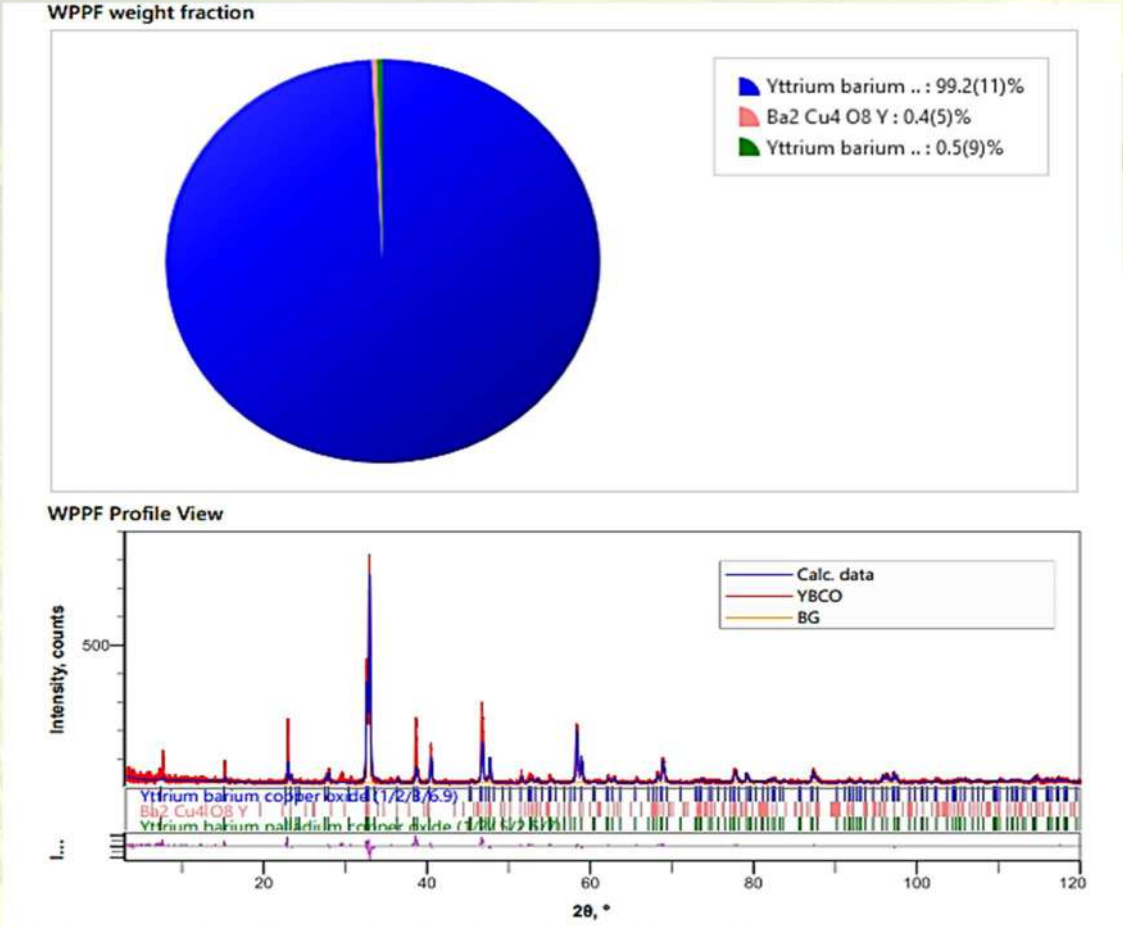


Figure 2. Quantitative confirmation of YBCO-(123) sample composition.

Our results confirmed that the sample is 99.21% pure based on the $YBa_2Cu_3O_{7-\delta}$ formula. A total of 0.45% structural change and 0.59% palladium element were seen in some parts of the sample. But these small defects did not negatively affect the conductivity of the sample.

The parameters of the crystal lattice of the $YBa_2Cu_3O_{6.91}$ sample synthesized by us were determined using the X-ray structural analysis method. The results are shown in the table above. The results show that our sample has an orthorhombic structure. This is a necessary factor to become a superconductor. You can see it in the picture below. (Fig. 3)

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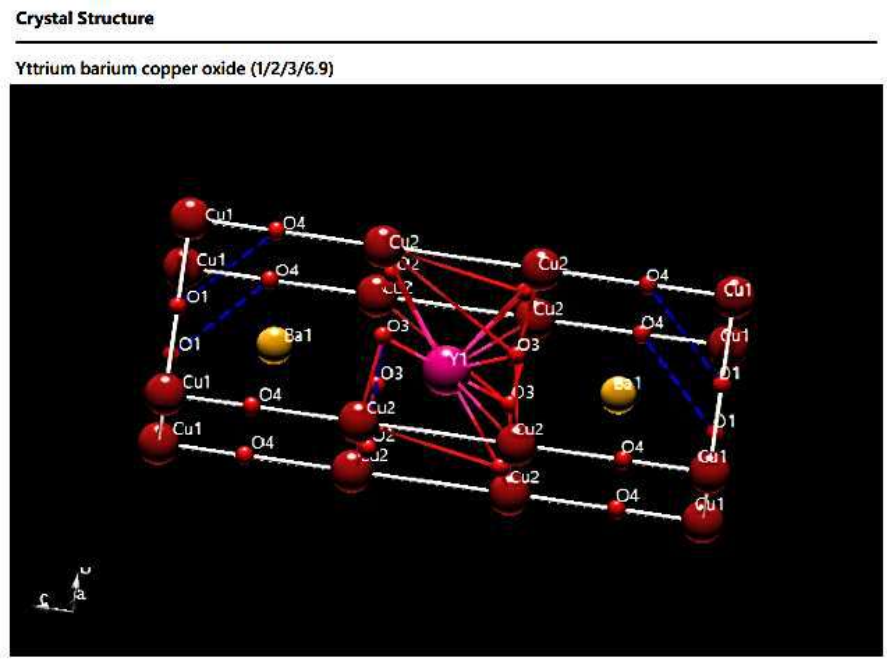


Figure 3. X-ray structural analysis of YBCO-123 crystal lattice

The appearance of the crystal lattice is orthorhombic, and it is made up to the maximum extent. Superconductivity occurs in the CuO layer around Y in the crystal lattice. The arrangement of the atoms in the nodes of the crystal lattice according to the coordinate axes is given in the following table. (Table 3).

Table 3.

YBCO crystal lattice parameters and interatomic distances.

Structure parameters

Element	x	y	z	Occ.	B	Charge	Multiplicity	Valence
Y1(Y)	0.500000	0.500000	0.500000	1.000	0.726	0	1	0.000
Ba1(Ba)	0.500000	0.500000	0.183930	1.000	0.979	0	2	0.000
Cu1(Cu)	0.000000	0.000000	0.000000	1.000	0.908	0	1	0.000
Cu2(Cu)	0.000000	0.000000	0.355010	1.000	0.726	0	2	0.000
O1(O)	0.000000	0.500000	0.000000	0.910	0.908	0	1	0.000
O2(O)	0.500000	0.000000	0.378190	1.000	0.816	0	2	0.000
O3(O)	0.000000	0.500000	0.376930	1.000	0.655	0	2	0.000
O4(O)	0.000000	0.000000	0.158400	1.000	1.005	0	2	0.000

The table shows the coordinate values of each atom in the YBCO-123 crystal lattice along the *x, y, z* axes. These values represent the spatial arrangement of the atoms considered to be constituents of the crystal lattice of the sample.

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Table 3.

The distance between the atoms of the crystal lattice.

Distance

Bond Def.	Distance, Å
Y1-Cu2(x,1+y,z)	3.21160
Y1-Cu2(1+x,y,z)	3.21160
Y1-Cu2(1+x,1-y,1-z)	3.21160
Y1-Cu2(x,1-y,1-z)	3.21160
Y1-Cu2(1+x,-y,1-z)	3.21160
Y1-Cu2(1+x,1+y,z)	3.21160
Y1-O2(x,1+y,z)	2.41165
Y1-O2	2.41165

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The table shows the distance between Y, the central atom of the crystal lattice, and the atoms located around it. It can be seen that Y and Cu atoms are located at the same distance.

Conclusion

As a result of the research, it was found that the correct formation of the crystal lattice depends on the temperature of sintering and calcination. Therefore, we sintered the sample at 940°C and then slowly cooled it to room temperature over 16 hours. Then it was observed that the structural structure of the sample was correctly formed by 99.21%.

The fact that the crystal lattice of the sample is orthorhombic is also shown in the above tables. This is the main factor of the YBCO-(123) sample's superconductivity property. The fact that the size of the crystal lattice took larger values compared to the world results also led to an increase in the critical temperature in our sample, i.e. up to Tc=100 K. This temperature is 5-6 K higher than the results obtained by world scientists.

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