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CRYSTAL STRUCTURE OF THE COMPOUND Ba_2GdRuO_6

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The work investigated the crystal structure of the double perovskite Ba_2GdRuO_6 by X-ray powder diffraction. X-ray phase analysis was performed, which confirmed the single-phase nature of the sample. Using the TREOR module of the HighScore Plus 3.0 program, the diffraction pattern was indexed and the space symmetry group I41/amd (141) of the tetragonal system with unit cell parameters a=b=2.478 Å, c=11.897 Å was determined. The microstructural parameters of the crystal lattice were refined using the Rietveld method using correlation matrices. The discrepancy factor is R=3.93%, which indicates the high quality of the structural model. The coordinates of the Ba, Gd, Ru, and O atoms in the structure were established, their Wyckoff positions and filling factors were determined. It is shown that the structure is a typical double perovskite $A_2BB'O_6$, where gadolinium (Gd^{3+}) and ruthenium (Ru^{5+}) atoms form regular octahedra with six oxygen atoms each, located in positions 8c and 8d, respectively, with a coordination number Z=6. Barium atoms occupy large cavities between the octahedra, and oxygen forms intermetallic bridges, ensuring the coherence of the structure. This structure is typical of materials with magnetic and electrical properties that are interesting for materials physics. Literature data on the magnetic, electronic, mechanical, and thermoelectric properties of Ba_2GdRuO_6 are analyzed. The material exhibits complex magnetic behavior with competition of antiferromagnetic and ferrimagnetic phases, a Curie temperature of 60 K, is a semiconductor with a band gap of about 1 eV, and exhibits high thermoelectric efficiency at elevated temperatures. The proposed crystal structure for the compound Ba2GdRuO6 can be determined in further studies using the diffraction spectrum recorded by the powder method with the Bragg-Brentano imaging geometry in a wider range. It is also possible to synthesize a single crystal of this compound and study the crystal structure by the single crystal method.

Key words: *Ba_2GdRuO_6, double perovskite, crystal structure, Rietveld method, X-ray diffraction, tetragonal syngony, magnetic properties.*

Заводянний В. В. Кристалічна структура сполуки Ba_2GdRuO_6

У роботі досліджено кристалічну структуру подвійного перовскіту Ba_2GdRuO_6 методом рентгенівської дифракції порошку. Проведено рентгенівський фазовий аналіз, який підтвердив однофазність зразка. За допомогою модуля TREOR програми HighScore Plus 3.0 виконано індексування дифрактограми та визначено просторову групу симетрії I41/amd (141) тетрагональної сингонії з параметрами елементарної комірки a=b=2.478 Å, c=11.897 Å. Методом Рітвельда уточнено мікроструктурні параметри кристалічної решітки з використанням кореляційних матриць. Фактор розбіжності становить R=3.93%, що свідчить про високу якість структурної моделі. Встановлено координати атомів Ba, Gd, Ru та O у структурі, визначено їх позиції Вікоффа та коефіцієнти заповнення. Показано, що структура є типовим подвійним перовскітом $A_2BB'O_6$, де атоми гадолінію (Gd^{3+}) та рутенію (Ru^{5+}) утворюють регулярні октаедри з шістьма атомами кисню кожен, розташовані в позиціях 8c та 8d відповідно з координаційним числом Z=6. Атоми барію займають великі порожнини між октаедрами, а кисень формує міжметалеві містки, забезпечуючи зв'язаність структури. Дана структура є типовою для матеріалів з магнітними та електричними властивостями, що є цікавими для фізики матеріалів. Проаналізовано літературні дані щодо магнітних, електронних, механічних та термоелектричних властивостей Ba_2GdRuO_6. Матеріал демонструє складну магнітну поведінку з конкуренцією антиферомагнітної та феримагнітної фаз, температурою Кюрі 60 K,

є напівпровідником з шириною забороненої зони близько 1 еВ та виявляє високу термоелектричну ефективність при підвищених температурах. Запропонована кристалічна структура для сполуки Ba_2GdRuO_6 може бути визначена в подальших дослідженнях за допомогою дифракційного спектру, відзнятого методом порошка з геометрією зйомки Брег-Брентано в більш широких межах. Також можна синтезувати монокристал цієї сполуки і дослідити кристалічну структуру методом монокристалу.

Ключові слова: *Ba_2GdRuO_6, подвійний перовскіт, кристалічна структура, метод Рітвельда, рентгенівська дифракція, тетрагональна сингонія, магнітні властивості.*

Introduction. Information on the crystal structure of inorganic compounds is an important aspect of research, which is closely related to the physical and chemical properties of materials, and significantly complements the information on the studied compounds. Analysis of recent studies and publications The key characteristics of Ba_2GdRuO_6 are given in [1]. The material exhibits complex magnetic behavior due to the competition between the antiferromagnetic (AFM) and ferrimagnetic (FiM) phases. GGA+U+SOC calculations show AFM as the ground state with a minimal energy advantage of only 11.39 meV over FiM. However, spin simulations reveal strong magnetic frustrations along the z-axis, which stabilize the FiM phase. The Curie temperature is 60 K, which is confirmed by magnetization measurements, which show a loss of saturation upon heating and a transition to a paramagnetic state. Electronic and magnetic structure The system is a semiconductor with a direct band gap of 1.04 eV (AFM) and 0.89 eV (FiM). The magnetic moments are distributed as follows: in the AFM configuration, the Gd(1-2)/Ru(1-2) ions have +6.9/+2.0 μB, while the Gd(3-4)/Ru(3-4) show -6.9/-2.0 μB. In the FiM state, all the Gd(1-4)/Ru(1-4) ions show +6.89/-2.0 μB. The Gd^{3+} ($4f^7$) and Ru^{4+} ($4d^4$) ions have specific electronic configurations with spin quantum numbers of 7/2 and 1, respectively. Gadolinium exhibits a fully filled f-shell with electrons in all seven orbitals, while ruthenium has the configuration $t_2g^3\uparrow$ $t_2g^1\downarrow$ e_g^0. Mechanical properties The material is mechanically stable according to the Born criteria. The Pugh coefficient indicates a ductile nature, and the positive Cauchy pressure of 66.53 GPa confirms the ionic nature of the chemical bonding in the structure. Thermoelectric properties The system exhibits hole-type conductivity with a positive Seebeck coefficient, reaching a maximum of 279 μV/K at 400 K. Most impressive is the high thermoelectric efficiency with a quality factor of 0.86 at 550 K even taking into account the lattice thermal conductivity. This makes Ba_2GdRuO_6 a promising candidate for thermoelectric energy conversion at elevated temperatures, as well as for spintronic applications due to its unique magnetic properties. In [2], the properties of this compound were investigated. In particular, using measurements of the susceptibility and surface resistance Ba_2GdRuO_6 and $Ba_2GdRu_{1-u}Cu_uO_6$, it was found that Gd, Ru and Cu are ordered antiferromagnetically at ~12.5 K, ~48 K and ~86 K, respectively. The electronic spin resonance of Gd is narrowed by exchange narrowing by paramagnetic Ru and broadened to almost undetectable below TN(Ru)=48 K. Ru does not resonate at all. Antiferromagnetic Cu exhibits microwave resonance in low fields. According to [3], new perovskites, $M2IILnIIIRuVO_6$, where MII = Ba and Sr, LnIII = rare earth elements, Y and Bi, were obtained. The Ba series exhibits cubic cells for LnIII = La to Dy and hexagonal cells for LnIII = Yb and Y. The Sr series exhibits superlattices for Ln = La to Nd and orthorhombic distortions for Ln = Sm to Yb. Ba_2LaRuO_6 has demonstrated catalytic activity and thermal stability for the reactions: $2NO + 2CO \rightarrow N_2 + 2CO_2$ and $2CO + O_2 \rightarrow 2CO_2$. The combination of three basic cations on Ru and the perovskite structure stabilize Ru in these catalysts. The authors of [4] conducted a search for microwave magnetic resonances of the Ru^{4+} and Ru^{5+} ions in a series of materials in which Ru is in octahedral coordination with six oxygen atoms. A number of ruthenates have been investigated, including RuO_2, $SrRuO_3$, $Sr_3Ru_2O_7$, $Ba_3Ru_2NiO_9$, Ba_2GdRuO_6, Sr_2YRuO_6 and Ba_2YRuO_6, which include paramagnetic, antiferromagnetic and ferromagnetic spin configurations. We present an analysis showing that the latter

material provides optimized detection of the Ru antiferromagnetic resonance for temperatures below TN=39 K; none were detected for frequencies up to 35 GHz in magnetic fields up to μoH=2 T. This result indicates that the energy band gap of the antiferromagnetic magnons exceeds the energy associated with the signal frequency. $SrRuO_3$ is a known ferromagnetic impurity phase in ruthenium cuprates. We report neutron diffraction measurements on $SrRuO_3$, revealing that it has a significant local moment at low temperatures, 1.25(0.1) μB; this moment disappears near 165 K. We show that it also does not exhibit ferromagnetic resonance, at least in the range 10–35 GHz. Diffraction and resonance studies have led to the conclusion that the reported ferromagnetic resonance in superconducting ruthenocuprates is actually due to the antiferromagnetically ordered Cu in these materials, and the presence of even a few percent of $SrRuO_3$ as a potential contaminant is of little importance. Research objective To propose a model of the crystal structure of the compound Ba_2GdRuO_6, and to refine the microstructural parameters by the Rietveld method based on the diffractogram taken by the powder method on X-ray copper filtered radiation with Bragg-Brentano imaging geometry and placed in the ICCD PDF-2 database for 2009 under the number 00-031-0140.

Presentation of the main material. To study the crystal structure of this compound, we made sure that the diffraction spectrum of the compound given in the ICCD PDF-2 database for 2009 is single-phase, using X-ray phase analysis. Using the HighScore Plus 3.0 TREOR program module, the X-ray pattern was indexed and the space symmetry group I41/amd (141) with lattice constants *a*=2.478A0, *b*=2.478A0, *c*=11.897A0 was selected. The microstructural parameters of the crystal lattice were refined using the Rietveld method, which are given in Table 1.

Table 1

Microstructural parameters of the crystal structure of the compound Ba_2GdRuO_6

Atom	Wyck.	s.o.f	*x/a*	*y/b*	*z/c*
Ba1	16h	1,0	0,0	0,08(2)	0,193(1)
Gd1	8c	1,0	0,0	0,0	0,0
Ru1	8d	1,0	0,0	0,0	0,5
O1	32i	1,0	-0,32(7)	0,0	0,54(2)
O2	16h	1,0	0,0	0,0	0,97(3)

The divergence factor R=3.93%.

The values of the interplanar distances and intensities are given in Table 2.

Table 2

The values of the interplanar distances and intensities given in the ICDD card and calculated for the structure of the compound Ba_2GdRuO_6

$2\theta_{cal}$	$2\theta_{obs}$	d_{cal}	d_{obs}	I_{cal}	I_{obs}	H	K	L
30,0052	30,0023(3)	2,97570	2,97599	100	100	0	0	4
37,0362	37,026(4)	2,42534	2,42596	3,40	2,03	0	1	1
43,0104	42,9821(6)	2,10128	2,10260	23,25	25,01	0	1	3
53,3322	53,3551(5)	1,71639	1,71571	27,17	35,20	0	1	5

The microstructural parameters of the compound lattice were refined using correlation matrices.

The proposed structural model is a double perovskite type $A_2BB'O_6$. Gadolinium atoms (Gd^{3+}) Fig. 1 and ruthenium (Ru^{5+}) Fig. 2 form regular octahedra with six oxygen atoms each.

The image of the crystal structure is shown in Fig. 3.

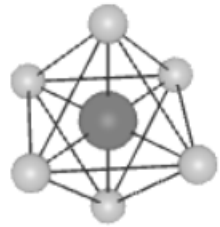

Fig. 1. Coordination polygon (octahedron) with a central gadolinium atom surrounded by six oxygen atoms

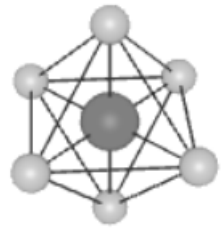

Fig. 2. Coordination polygon (octahedron) with a central ruthenium atom surrounded by six oxygen atoms

Gadolinium is a rare earth element occupying the 8c position with a coordination number of Z=6. Ruthenium is a transition metal occupying the 8d position and has a coordination number of Z=6. Barium is an alkaline earth metal occupying large cavities between octahedra. Oxygen atoms form bridges between the metals, ensuring the coherence of the structure.

This structure is typical of materials with magnetic and electrical properties that are interesting for materials physics.

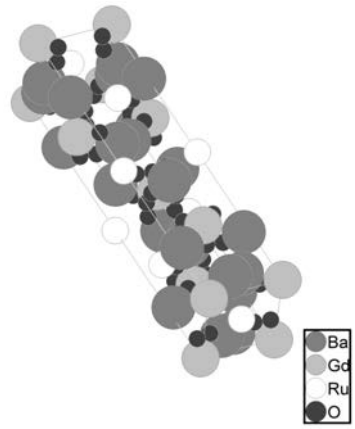

Fig. 3. Crystal structure of the compound Ba2GdRuO6

Conclusions and prospects for further research. We have proposed a crystal structure for the compound Ba2GdRuO6. The crystal structure of the compound belongs to the tetragonal system, the space symmetry group I41/amd (141) with lattice constants a=2.478A^0, b=2.478A^0, c=11.897A^0. The microstructural parameters of the compound were refined by the Rietveld method using correlation matrices and are given in this work. Gadolinium and ruthenium atoms form octahedra with six oxygen atoms. The crystal structure of this compound can be studied in further studies for a wider diffraction spectrum or by the single crystal method.

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