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## Synthesis and crystal structure of two-slab $Ba_{1-x}Sr_xNd_2In_2O_7$ indates

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The conditions of isovalent substitution of Ba atoms by Sr atoms in the A-position of the  $BaNd_2In_2O_7$  two-slab perovskite-like structure of  $Ba_{1-x}Sr_xNdIn_2O_7$  type are established:  $0 \leq x \leq 0.22$ . The tetragonal ( $P4_2/mmm$ ) crystal structure of  $Ba_{1-x}Sr_xNdIn_2O_7$  indates with  $x = 0.1$  and  $0.2$  was determined by the Rietveld method.  $Ba_{1-x}Sr_xNdIn_2O_7$  structure is based on two-dimensional (infinite in the XY plane) perovskite-like blocks of two slabs connected by vertices of deformed  $InO_6$  octahedra. Neighboring blocks are separated by a slab of  $NdO_9$  polyhedra and interconnected by O – Nd – O bonds. It is found that isovalent substitution of Ba atoms by Sr atoms reduces the Nd – O2 interblock distance, which brings the structure of two-dimensional slab structure closer to the structure of three-dimensional perovskite and is one of the main factors of destruction of  $Ba_{1-x}Sr_xNdIn_2O_7$  slab structure at  $x > 0.22$ .

**Keywords:** compounds of  $A_{n+1}B_nO_{3n+1}$  type, slab perovskite-like structure, interblock distance, polyhedron deformation.

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### Introduction

Representatives of the  $A_{n+1}B_nO_{3n+1}$  family of compounds with a slab perovskite-like structure (SPS) are distinguished by an extremely wide range of physicochemical properties, which includes, in particular, significant magnetoresistance, conductive, ion exchange and luminescent properties etc. [1-8]. These characteristics of  $A_{n+1}B_nO_{3n+1}$  compounds are caused by the features of their SPS, in which perovskite-like blocks of  $n$  slabs of  $BO_6$  octahedra connected by vertices are interspersed with layers of  $AO_9$  polyhedra [1, 9-15].

Deformation of crystal structure belongs to the factors that significantly affect the properties of oxide functional materials. Among the members of the  $A_{n+1}B_nO_{3n+1}$  Ruddlesden-Popper family a significant dimensional discrepancy between A and B sublattices of the SPS occurs in two-slabs  $BaLn_2In_2O_7$  indates ( $Ln = La - Nd$ ).  $Ln^{3+}$  cations ( $LnO_9$  polyhedra) are placed in the A position of SPS of these compounds,  $In^{3+}$  large cations ( $InO_6$  octahedra) and  $Ba^{2+}$  ( $BaO_{12}$  cuboctahedra) are placed in the B position of SPS [11,12].

Isomorphous substitutions of atoms in their structure

are one of the ways to regulate the deformation of SPS and, accordingly, the properties of compounds and phases of the  $A_{n+1}B_nO_{3n+1}$  type.  $BaNd_2In_2O_7$  indate is of the greatest interest from the point of view of the magnitude of dimensional mismatch of A- and B-sublattices. However, at present there are no data on isomorphous substitutions impact on the structure of SPS phases based on it.

The aim of this work is to determine the effect of isovalent substitution of Ba atoms in SPS of the  $BaNd_2In_2O_7$  on the structure features of the two-slabs SPS of  $Ba_{1-x}Sr_xNd_2In_2O_7$  indates.

### I. Materials and methods

Samples of  $Ba_{1-x}Sr_xNd_2In_2O_7$  were synthesized by co-crystallization (evaporation with vigorous stirring) of a mixture of aqueous solutions of barium acetate and nitrates of strontium, neodymium and indium with a ratio of Ba : Sr : Nd : In =  $1 - x : x : 2 : 2$  followed by heat treatment of a product obtained on a gas burner to remove the bulk of nitrogen oxides. The charge obtained was

pressed into disks and subjected to multistage heat treatment at 1570 K (with grinding and pressing of samples after each stage of heat treatment) to achieve a constant phase composition. Barium acetate and strontium, neodymium and indium nitrates of “chemical pure” brands were used as raw (initial) materials.

X-ray diffraction spectra of polycrystalline samples were detected on a Shimadzu XRD-6000 diffractometer in a discrete mode (scanning step  $0.02^\circ$ , exposure at a point of 5 seconds, angle interval  $2\theta = 15 - 67^\circ$ ) on a  $\text{CuK}\alpha$  filtered (arc graphite monochromator) radiation. The crystal structure of samples obtained was determined by the Rietveld method. Primary processing of diffraction spectra and structural calculations were performed using a hardware-software complex, as described in [16].

## II. Experimental results

X-ray diffraction study of the limits of isovalent substitution of Ba by Sr atoms in the  $\text{BaNd}_2\text{In}_2\text{O}_7$  SPS have shown the existence of a rather narrow region ( $0 \leq x \leq 0.22$ ) of  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  indates with SPS (Fig. 1), in contrast to that for  $\text{Ba}_{1-x}\text{Sr}_x\text{La}_2\text{In}_2\text{O}_7$  indates ( $0 \leq x \leq 0.75$ ) [14]. Probable reason for the lower isomorphous capacity of  $\text{BaNd}_2\text{In}_2\text{O}_7$  SPS compared to  $\text{BaLa}_2\text{In}_2\text{O}_7$  SPS is the increase in the dimensional mismatch of the A- and B-sublattices of  $\text{BaLn}_2\text{In}_2\text{O}_7$  SPS with RE atom size decreasing. Samples of  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  with  $x = 0.3$  and  $0.4$  are not single-phase and contain a number of additional phases, the main of which is the phase with perovskite structure (likely, based on  $\text{NdInO}_3$ ).

To study the impact of isovalent substitution of Ba atoms on the features of SPS the  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  indates of  $x = 0.1$  and  $0.2$  composition were selected. X-ray diffraction spectra of  $\text{Ba}_{0.9}\text{Sr}_{0.1}\text{Nd}_2\text{In}_2\text{O}_7$  and  $\text{Ba}_{0.8}\text{Sr}_{0.2}\text{Nd}_2\text{In}_2\text{O}_7$  are similar to those of two-slabs  $\text{BaNd}_2\text{In}_2\text{O}_7$  [11], and their indexing has shown that SPS of  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  ( $x = 0.1$  and  $0.2$ ) belongs to tetragonal crystal system. Systematics extinctionson on diffraction patterns indicates the following possible spatial groups: centrosymmetric  $P4_2/mnm$  or  $P4n2$  and  $P4_2nm..$  Test for

the generation of the second harmonic signal IAG: Nd laser showed that the relative intensity of signal  $I_{2\omega}$  for  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  with  $x = 0.1$  and  $0.2$  does not exceed  $0.01 I_{2\omega}$  for noncentrosymmetric compound  $\text{La}_4\text{Ti}_4\text{O}_{14}$  with SPS. This value of  $I_{2\omega}$  definitely indicates that their crystal structure belongs to  $P4_2/mnm$  centrosymmetric spatial group.

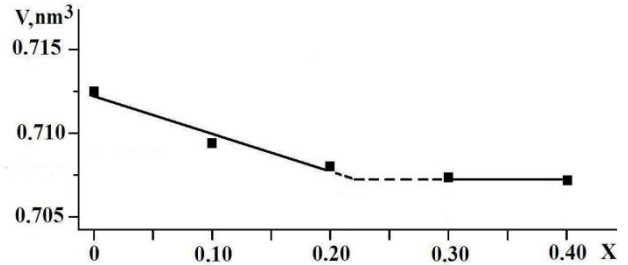


Fig. 1. Dependence of unit cell volume for  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  indates with SPS on the substitution degree of Ba atoms ( $x$  values).

Taking into account the similarity of the diffraction patterns of  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  indates of SPS and  $\text{BaNd}_2\text{In}_2\text{O}_7$  indate, the primary estimation of the coordinate parameters of atoms for the initial models of  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  structures was performed according to known structural data for two-slabs  $\text{BaNd}_2\text{In}_2\text{O}_7$  [11] ( $P4_2/mnm$  (136) space group) with the localization of large Ba and Sr atoms in the center of perovskite block in  $(\text{Ba,Sr})\text{O}_{12}$  polyhedra, and smaller Nd atoms on the block boundary in  $\text{NdO}_9$  polyhedra. Comparison of experimental and calculated peak intensities for these structure models showed their satisfactory coincidence.

The results of refining the coordinate and thermal parameters of the structures of isovalently substituted  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  indates and other structural data are presented in Fig. 2 and listed in Table 1. The refined  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  indates compositions are correspond to the experimentally set within the error of determination.

The main structural units of  $\text{Ba}_{1-x}\text{Sr}_x\text{Nd}_2\text{In}_2\text{O}_7$  ( $x = 0.1$  and  $0.2$ ) SPS are two-dimensional (infinite in the XY plane) perovskite-like blocks, each of which consists of two slabs of deformed  $\text{InO}_6$  octahedra (Fig. 3, a). In blocks

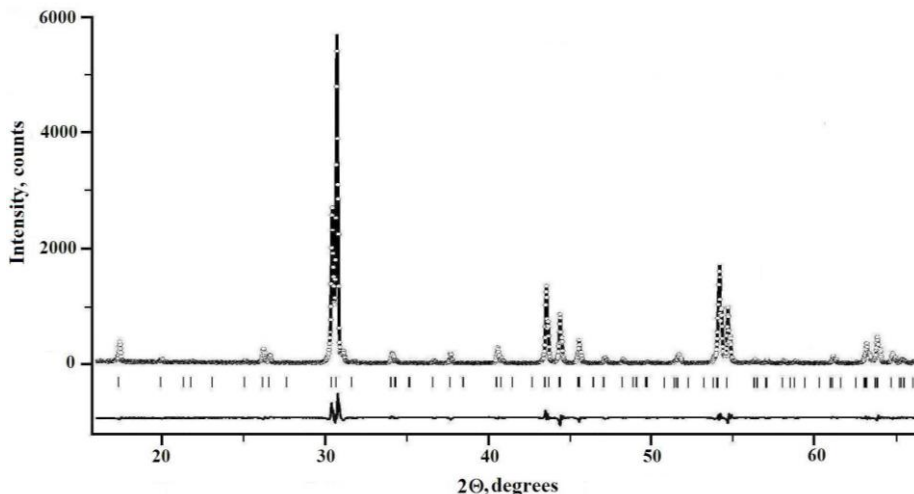


Fig. 2. Experimental (circles), calculated (solid) and difference (the lowest line) diffraction pattern of  $\text{Ba}_{0.8}\text{Sr}_{0.2}\text{Nd}_2\text{In}_2\text{O}_7$  indate ( $\text{CuK}\alpha$  radiation).

Table 1

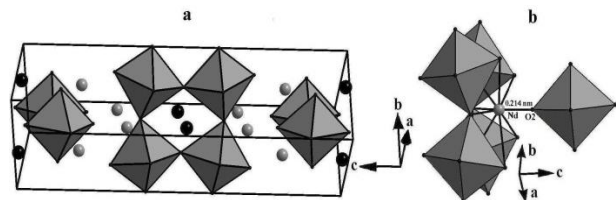
Crystallographic data for  $Ba_{1-x}Sr_xNd_2In_2O_7$  with SPS.

Atom	Position	$Ba_{0.9}Sr_{0.1}Nd_2In_2O_7$				$Ba_{0.8}Sr_{0.2}Nd_2In_2O_7$			
		*	X	Y	Z	*	X	Y	Z
Ba	4f	0.9	0.2511(2)	0.2511(2)	0	0.8	0.2489(2)	0.2489(2)	0
Sr		0.1				0.2			
Nd	8j	1	0.2738(2)	0.2738(2)	0.1858(2)	1	0.2735(2)	0.2735(2)	0.1865(2)
In	8j	1	0.2660(2)	0.2660(2)	0.3980(3)	1	0.2681(3)	0.2681(3)	0.3961(3)
O1	4g	1	0.775(3)	0.225(3)	0	1	0.775(2)	0.225(2)	0
O2	8j	1	0.180(2)	0.180(2)	0.285(3)	1	0.181(3)	0.181(3)	0.284(3)
O3	8h	1	0	0.5	0.107(2)	1	0	0.5	0.113(2)
O4	4e	1	0	0	0.129(2)	1	0	0	0.130(2)
O5	4e	1	0	0	0.397(3)	1	0	0	0.400(3)
Space group		$P4_2/mnm$ (136)				$P4_2/mnm$ (136)			
Parameters of crystal lattice (nm)		$a = 0.58891(5)$ $c = 2.0454(3)$				$a = 0.58864(4)$ $c = 2.0434(2)$			
Independent reflections		86				86			
Total isotropic factor. $B$ ( $nm^2$ )		$0.25(6) \cdot 10^{-2}$				$0.42(9) \cdot 10^{-2}$			
Texture parameter		0.911(9) [001] texture axis				0.71(1) [001] texture axis			
Reliability factor. $R_w$		0.043				0.061			

\*– position filling

$InO_6$  octahedra are connected only by vertices and each octahedron has five common vertices with adjacent octahedra of the same block. In the diagonal direction of XY plane, the adjacent blocks are offset relative to each other by half an edge of the perovskite cube and alternate along Z axis.

Adjacent perovskite-like blocks in  $Ba_{1-x}Sr_xNd_2In_2O_7$  SPS are separated by a slab of  $NdO_9$  polyhedra and held together by – O – Nd – O – interblock bonds. Eight of the nine oxygen atoms of  $NdO_9$  polyhedron (four O2, two O3, one O4, and one O5) belong to the same block as the Nd atoms, and one oxygen atom (O2) belongs to the adjacent block (Fig. 3, b). The length of the specified Nd – O2 interblock bond (0.217(2) – 0.214(1) nm) is the smallest of all bonds of  $NdO_9$  polyhedron, and its length is close to the minimum known Nd – O distances. This fact indicates the impossibility of finding significantly greater Ba and Sr atoms (than Nd atoms) in  $Ba_{1-x}Sr_xNd_2In_2O_7$  SPS at 8j position in  $MeO_9$  polyhedra between perovskite-like blocks and correlates with the data of Refs. [11, 12] on the completely ordered nature of the distribution of Ba and REE atoms in  $BaLn_2In_2O_7$  with SPS.



**Fig. 3.** Crystal structure of  $Ba_{0.9}Sr_{0.1}Nd_2In_2O_7$  in the form of  $InO_6$  octahedra and Ba and Sr atoms (black circles) and Nd atoms (grey circles) (a); the structure of the interblock boundary in the  $Ba_{0.8}Sr_{0.2}Nd_2In_2O_7$  with SPS in the form of  $InO_6$  octahedra and Nd atoms (grey circle) (b).

It should be noted that two O2 atoms of nine oxygen atoms of  $NdO_9$  polyhedron are located at much greater

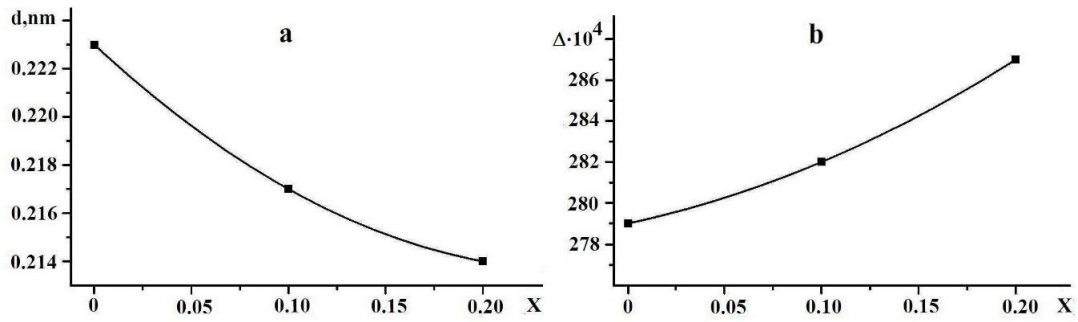
distances (0.356(3) – 0.355(2) nm (Table 2)) from Nd atom. Therefore the coordination number of central atoms in  $NdO_9$  polyhedron can be considered as 1 + 6 + 2 taking into account the presence of one the shortest Nd – O2 interblock bond.

Ba and Sr atoms in  $Ba_{1-x}Sr_xNd_2In_2O_7$  with SPS are located only in 4f position in great intrablock voids of the perovskite-like block, where their coordination polyhedron is a deformed (Ba,Sr) $O_{12}$  cuboctahedron.

Analysis of the data obtained in this paper on the structure of  $Ba_{1-x}Sr_xNd_2In_2O_7$  ( $x = 0.1$  and  $0.2$ ) indates and data of Ref. [11] on  $BaNd_2In_2O_7$  indate has revealed that the gradual replacement of Ba by Sr atoms in  $AO_{12}$  cuboctahedron of perovskite block of SPS leads to Nd – O2 intrablock distance decreasing (approaching of adjacent perovskite-like blocks to each other) and to the degree of  $InO_6$  octahedra deformation increasing (Fig. 4a, Table 2). The values of  $NdO_9$  polyhedra deformation degree are slightly increased with substitution degree of Ba atoms increasing (Fig. 4, b). However, it should be noted that the meaning of  $\Delta NdO_9$  is already one of the greatest among the Ruddlesden-Popper family compounds even for unsubstituted  $BaNd_2In_2O_7$ .

Reducing the distance between two-slab perovskite-like blocks brings the structure of two-dimensional SPS closer to the structure of three-dimensional, thermodynamically more stable perovskite, which leads to destabilization of SPS and gives reasons to conclude that this factor limits the region of  $Ba_{1-x}Sr_xNd_2In_2O_7$  with SPS solid solutions and the absence of  $SrNd_2In_2O_7$  compound with SPS. The above is confirmed by the appearance of a phase with perovskite structure in non-single-phase samples of  $Ba_{1-x}Sr_xNd_2In_2O_7$  with  $x > 0.22$ .

Obviously, the increase in deformation degree of  $InO_6$  octahedra in  $Ba_{1-x}Sr_xNd_2In_2O_7$  SPS with increase of the degree of isovalent substitution is caused by different sizes of  $Sr^{2+}$  cation (0.158 nm) compared to  $Ba^{2+}$  cation (0.175 nm) [17].



**Fig. 4.** Dependences of the length of Nd - O2 interblock bond (a) and the deformation degree of NdO<sub>9</sub> interblock polyhedra (b) in Ba<sub>1-x</sub>Sr<sub>x</sub>Nd<sub>2</sub>In<sub>2</sub>O<sub>7</sub> with SPS on the substitution degree of Ba atoms (x).

**Table 2**

Interatomic distances (nm), deformation degree ( $\Delta$ ) of  $MeO_n$  polyhedra in Ba<sub>1-x</sub>Sr<sub>x</sub>Nd<sub>2</sub>In<sub>2</sub>O<sub>7</sub> (x = 0, 0.1 and 0.2) SPS.

BaNd <sub>2</sub> In <sub>2</sub> O <sub>7</sub> [11]		Ba <sub>0.9</sub> Sr <sub>0.1</sub> Nd <sub>2</sub> In <sub>2</sub> O <sub>7</sub>		Ba <sub>0.8</sub> Sr <sub>0.2</sub> Nd <sub>2</sub> In <sub>2</sub> O <sub>7</sub>	
BaO <sub>12</sub> polyhedron		(Ba <sub>0.9</sub> Sr <sub>0.1</sub> )O <sub>12</sub> polyhedron		(Ba <sub>0.8</sub> Sr <sub>0.2</sub> )O <sub>12</sub> polyhedron	
Atom-atom	Distances	Atom-atom	Distances	Atom-atom	Distances
Ba – 2O1	0.286(3)	Ba – 2O1	0.281(2)	Ba – 2O1	0.279(2)
Ba – 4O3	0.306(2)	Ba – 4O3	0.302(1)	Ba – 4O3	0.311(2)
Ba – 2O5	0.295(2)	Ba – 2O5	0.296(2)	Ba – 2O5	0.292(2)
Ba – 2O1	0.306(3)	Ba – 2O1	0.309(1)	Ba – 2O1	0.310(2)
Ba – 2O4	0.342(1)	Ba – 2O4	0.337(3)	Ba – 2O4	0.337(3)
Ba – O <sub>aver.</sub>	0.307	(Ba <sub>0.9</sub> Sr <sub>0.1</sub> ) – O <sub>aver.</sub>	0.305	(Ba <sub>0.8</sub> Sr <sub>0.2</sub> ) – O <sub>aver.</sub>	0.307
$\Delta$	32·10 <sup>-4</sup>	$\Delta$	31·10 <sup>-4</sup>	$\Delta$	35·10 <sup>-4</sup>
NdO <sub>9</sub> polyhedron		NdO <sub>9</sub> polyhedron		NdO <sub>9</sub> polyhedron	
Nd – 1O2*	0.223(2)	Nd – 1O2*	0.217(2)	Nd – 1O2*	0.214(1)
Nd – 1O5	0.248(1)	Nd – 1O5	0.253(2)	Nd – 1O5	0.258(1)
Nd – 2O2	0.247(1)	Nd – 2O2	0.248(1)	Nd – 2O2	0.249(2)
Nd – 1O4	0.258(1)	Nd – 1O4	0.256(2)	Nd – 1O4	0.255(2)
Nd – 2O3	0.262(3)	Nd – 2O3	0.264(3)	Nd – 2O3	0.257(1)
Nd – 2O2	0.356(2)	Nd – 2O2	0.356(3)	Nd – 2O2	0.355(2)
Nd – O <sub>aver.</sub>	0.273	Nd – O <sub>aver.</sub>	0.274	Nd – O <sub>aver.</sub>	0.272
$\Delta$	279·10 <sup>-4</sup>	$\Delta$	282·10 <sup>-4</sup>	$\Delta$	287·10 <sup>-4</sup>
InO <sub>6</sub> polyhedron		InO <sub>6</sub> polyhedron		InO <sub>6</sub> polyhedron	
In – 1O4	0.210(1)	In – 1O4	0.203(2)	In – 1O4	0.200(1)
In – 2O3	0.209(2)	In – 2O3	0.209(1)	In – 2O3	0.210(1)
In – 1O1	0.210(1)	In – 1O1	0.209(1)	In – 1O1	0.212(2)
In – 1O5	0.215(2)	In – 1O5	0.222(2)	In – 1O5	0.223(2)
In – 1O2	0.236(2)	In – 1O2	0.242(2)	In – 1O2	0.240(1)
In – O <sub>aver.</sub>	0.215	In – O <sub>aver.</sub>	0.216	In – O <sub>aver.</sub>	0.216
$\Delta$	20·10 <sup>-4</sup>	$\Delta$	37·10 <sup>-4</sup>	$\Delta$	35·10 <sup>-4</sup>

\*– interblock distance.

It should be noted that the addition of Sr atoms into BaNd<sub>2</sub>In<sub>2</sub>O<sub>7</sub> SPS does not change the syngony type and the spatial group of the initial unsubstituted compound, while there is a decrease in syngony to rhombic (*Fmmm*) in the Ba<sub>1-x</sub>Sr<sub>x</sub>La<sub>2</sub>In<sub>2</sub>O<sub>7</sub> indates [14]. However, for both Ba<sub>1-x</sub>Sr<sub>x</sub>Ln<sub>2</sub>In<sub>2</sub>O<sub>7</sub> (Ln = La, Nd) solid solutions there is a similar nature of the effect of Ba atoms on Sr atom substitution on the parameters of (Ba,Sr)O<sub>12</sub>, LnO<sub>9</sub> and InO<sub>6</sub> polyhedra.

## Conclusions

Thus, in this paper the conditions of isovalent substitution of Ba atoms in BaNd<sub>2</sub>In<sub>2</sub>O<sub>7</sub> indate of Ba<sub>1-x</sub>Sr<sub>x</sub>Nd<sub>2</sub>In<sub>2</sub>O<sub>7</sub> type have established (0 ≤ x ≤ 0.22), the structure of Ba<sub>1-x</sub>Sr<sub>x</sub>Nd<sub>2</sub>In<sub>2</sub>O<sub>7</sub> indates with SPS with substitution degree of Ba atoms x = 0.1 and 0.2 has determined. Analysis of the data obtained has revealed the

structural factors that limit the area of SPS existing in the  $Ba_{1-x}Sr_xNd_2In_2O_7$  system and has defined the composition – crystal structure features relationship of  $Ba_{1-x}Sr_xNd_2In_2O_7$  indates with SPS, which can be used to regulate their structurally dependent properties.

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## Синтез та кристалічна структура двошарових індатів $Ba_{1-x}Sr_xNd_2In_2O_7$

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Одним із основних завдань сучасного матеріалознавства є дослідження впливу ізоморфних заміщень атомів на кристалічну структуру та властивості оксидних сполук. Дана робота присвячена дослідженню заміщення атомів Ва меншими атомами Sr в двошаровій перовськітоподібній структурі  $BaNd_2In_2O_7$  та його впливу на особливості будови синтезованих індатів  $Ba_{1-x}Sr_xNd_2In_2O_7$ . Представлені результати досліджень одержаних фаз методами рентгенівської порошкової дифрактометрії та результати визначення їх кристалічної структури методом Рітвельда. Встановлена область існування твердих розчинів  $Ba_{1-x}Sr_xNd_2In_2O_7$  з двошаровою перовськітоподібною структурою ( $0 \leq x \leq 0,22$ ) та визначені координати атомів для індатів з  $x = 0,1$  і  $x = 0,2$ . Встановлені кореляції між ступенем заміщення атомів Ва, довжиною міжблокової відстані Nd – O2 та ступенями деформації октаєдрів  $InO_6$  і полієдрів  $NdO_9$ . Показано, що такий тип заміщення призводить до зменшення довжини міжблокового зв'язку Nd – O2 (з 0,223(2) нм при  $x = 0$  до 0,214(1) нм при  $x = 0,2$ ). Це наближує будову двовимірної структури  $Ba_{1-x}Sr_xNd_2In_2O_7$  до тривимірної структури перовскіту та призводить до її руйнування при  $x > 0,22$ .

**Ключові слова:** сполуки типу  $A_{n+1}B_nO_{3n+1}$ , шарувата перовськітоподібна структура, міжблокова відстань, деформація полієдрів.