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Data Article

Data supporting the results of the characterization of the phases and structures appearing during the synthesis process of $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ by auto-combustion

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ABSTRACT

The data presented has to do with identifying the various phases arising during the synthesis of the Y-type hexaferrite series $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ by auto-combustion that we deem important for their microstructural and magnetic properties. The data and the related analyses support the research paper "Ni-substitution effect on the properties of $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ powders" [1]. Thus, the parameters are presented of the phases appearing after auto-combustion and after the initial annealing at 800 °C, namely, crystal cell and crystallite size. Also, additional data are provided obtained by EDS concerning the Ba:Sr:Zn:Ni:Fe ratio in $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ ($x = 0.8$, 1, 1.5) samples synthesized at 1170 °C for 10 h. The data can be used as a reference in establishing how the phases distinguished during the initial process of auto-combustion affect the $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ powders, which are candidates for

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room-temperature multiferroic materials. The data have not been published previously and are made available to permit critical or further analyses.

Specifications Table

Subject	Materials Science, Electronic, Optical and Magnetic Materials
Specific subject area	Multiferroic Materials, Hexaferrites, Sol-Gel Auto-Combustion
Type of data	Tables Figures Text file
How data were acquired	X-ray diffraction (XRD) measurements performed using a Brucker D8 diffractometer Scanning electron microscopy and energy dispersive X-ray spectroscopy (FEI XL30 FEG-ESEM, Bruker Quantax EDS coupled to ESEM)
Data format	Raw Analyzed Filtered
Parameters for data collection	The characterization was implemented by X-ray diffraction (XRD) carried out by a Brucker D8 diffractometer (40 kV, 30 mA) controlled by DIFFRACTPLUS software in Bragg-Brentano reflection geometry with Cu-Kα radiation ($\lambda = 1.5418$ Å); and by scanning electron microscopy and energy dispersive X-ray spectroscopy (FEI XL30 FEG-ESEM, Bruker Quantax EDS coupled to ESEM).
Description of data collection	The XRD experiments were conducted on powder samples. The percentage, crystal cell parameters and crystallite size of the phases were determined from X-ray diffractograms. The EDS analyses were performed on four points on polished cross-sections of bulk samples (pellets) in view of finding the Ba:Sr:Zn:Ni:Fe ratio.
Data source location	Institution: Institute of Electronics, Bulgarian Academy of Sciences City: Sofia Country: Bulgaria Institution: Institute of General and Inorganic Chemistry City: Sofia Country: Bulgaria Institution: Greenmat, Chemistry Department, University of Liege, City: Liège Country: Belgium
Data accessibility	With the article
Related research article	T. Koutzarova, S. Kolev, K. Krezhov, B. Georgieva, Ch. Ghelev, D. Kovacheva, B. Vertruyen, R. Closset, L. M. Tran, M. Babij, A. J. Zaleski, Ni-substitution effect on the properties of $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ powders, J. Magn. Magn. Mater. doi: 10.1016/j.jmmm.2020.166725

Value of the Data

- The data distinguishes the intermediate phases appearing during the synthesis of a Y-type hexaferrite ($Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$) by auto-combustion;
- The EDS analysis yields reliable information on the chemical composition at different points on bulk $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ samples;
- The data could be useful in identifying the phases and their effect during the synthesis of other hexaferrites;
- The data supplies important additional information to the related research article.

Table 1
Phase percentage, crystal cell parameters and average crystallite size obtained from the XRD patterns of auto-combusted powders and powder annealed at 800 °C for three hours.

Sample	Spinel	$(Ba,Sr)CO_3$	$(Ba,Sr)FeO_{3-x}$	$BaSrFe_4O_8$
$Ba_{0.5}Sr_{1.5}Zn_{1.2}Ni_{0.8}Fe_{12}O_{22}$				
auto-combusted powder	87%	13%		
percentage	8.378(6) Å	5.099(4) Å		
a	10 nm	8.624(9) Å		
b		6.098(4) Å		
c		19 nm		
crystallite size				
$Ba_{0.5}Sr_{1.5}Zn_{1.2}Ni_{0.8}Fe_{12}O_{22}$				
annealed at 800°C	65%		25%	10%
percentage	8.395(5) Å		5.664(1) Å	5.435(5) Å
a	11 nm		21.681(4) Å	8.055(5) Å
b			5 nm (fix)	79 nm
c				
crystallite size				
$Ba_{0.5}Sr_{1.5}ZnNiFe_{12}O_{22}$	87%	13%		
auto-combusted powder	8.371(1) Å	5.098(2) Å		
percentage	11 nm	8.621(8) Å		
a		6.105(5) Å		
b		19 nm		
c				
crystallite size				
$Ba_{0.5}Sr_{1.5}ZnNiFe_{12}O_{22}$				
annealed at 800°C	68%		27%	5%
percentage	8.385(1) Å		5.685(4) Å	5.446(2) Å
a	12 nm		21.860(3) Å	8.071(6) Å
b			5 nm (fix)	24 nm
c				
crystallite size				
$Ba_{0.5}Sr_{1.5}Zn_{0.5}Ni_{1.5}Fe_{12}O_{22}$	88%	12%		
auto-combusted powder	8.357(8) Å	5.101(0) Å		
percentage	9 nm	8.601(6) Å		
a		6.097(6) Å		
b		21 nm		
c				
crystallite size				
$Ba_{0.5}Sr_{1.5}Zn_{0.5}Ni_{1.5}Fe_{12}O_{22}$				
annealed at 800°C	67%		27%	6%
percentage	8.368(1) Å		5.659(0) Å	5.437(0) Å
a	10 nm		21.740(4) Å	8.052(9) Å
b			5 nm (fix)	79 nm
c				
crystallite size				

1. Data description

The data and analyses included here corroborate the results of and the conclusions drawn from the study of $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ (x = 0.8, 1, and 1.5) hexaferrites synthesized by sol-gel auto-combustion [1]. The XRD analysis was employed to distinguish between the phases formed during the consecutive steps of the synthesis of $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ (x = 0.8, 1, and 1.5). Fig. 1 shows the XRD patterns of the auto-combusted powders and the powder treated at 800 °C for three hours for samples with x = 1, and 1.5. The corresponding XRD patterns for sample $Ba_{0.5}Sr_{1.5}Zn_{1.2}Ni_{0.8}Fe_{12}O_{22}$ are presented in Koutzarova et al. [1]. A spinel-type phase (Ni-Zn mixed ferrite (Zn, Ni)Fe_2O_4) and (Ba, Sr)CO_3 were observed in the as-synthesized auto-combustion powders. The XRD-patterns of the powders heat-treated at 800 °C exhibit the peaks of spinel type phase $BaFeO_{3-x}$ and $BaSrFe_4O_8$. Table 1 summarizes the data for the crystal cell

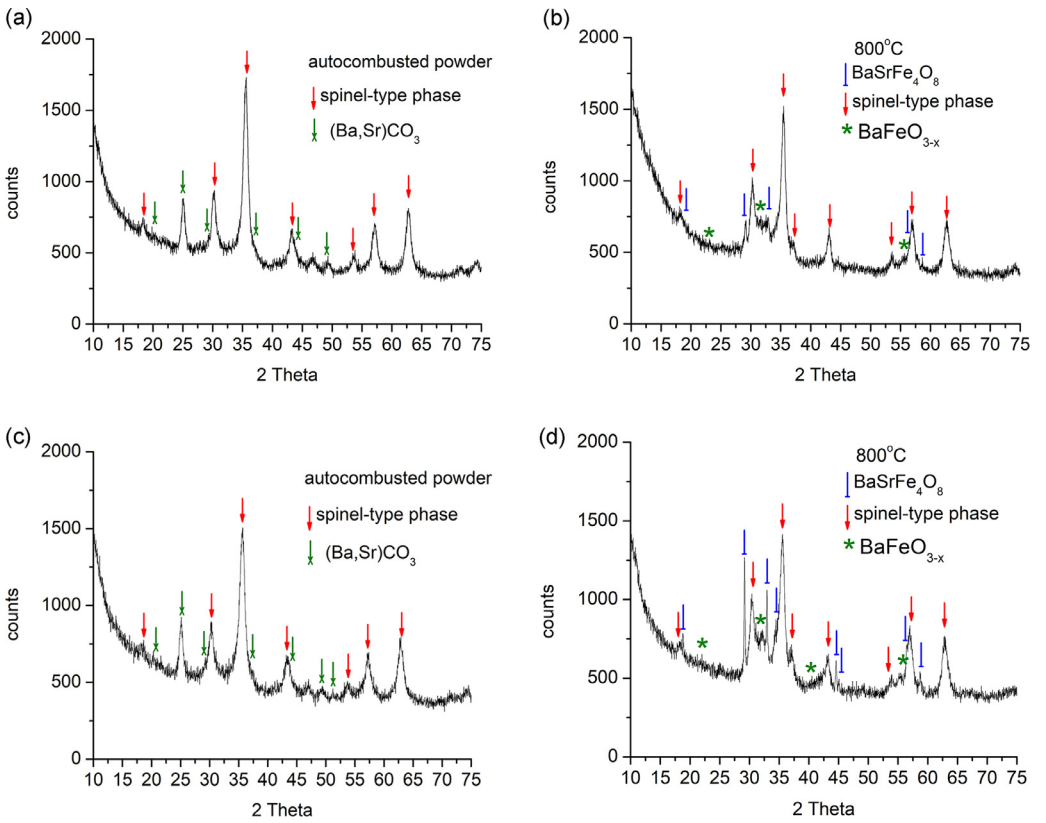

Fig. 1. XRD-patterns of auto-combusted powders (a, c) and powder annealed at 800 °C for three hours (b, d) for samples x = 1 (a, b), and 1.5 (c, d).

Table 2
The Ba:Sr:Zn:Ni:Fe ratio estimated from the EDX analyses of $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_{ix}Fe_{12}O_{22}$ (x = 0.8, 1, 1.5) samples at the four points on polished cross-sections surface.

Sample	$Ba_{0.5}Sr_{1.5}Zn_{1.2}Ni_{0.8}Fe_{12}O_{22}$ Ba:Sr:Zn:Ni:Fe	$Ba_{0.5}Sr_{1.5}ZnNiFe_{12}O_{22}$ Ba:Sr:Zn:Ni:Fe	$Ba_{0.5}Sr_{1.5}Zn_{0.5}Ni_{1.5}Fe_{12}O_{22}$ Ba:Sr:Zn:Ni:Fe
Point 1	0.5:1.5:1.1:0.8:12.3	0.5:1.7:1.7:1.7:16.7	0.5:1.5:0.5:1.4:12.9
Point 2	0.5:1.6:1.2:0.7:12.4	0.5:1.5:1.8:1.5:16.6	0.5:1.5:0.5:1.3:12.0
Point 3	0.5:1.5:1.1:0.8:12.4	0.5:1.7:1.1:1.0:12.3	0.5:1.7:0.5:1.3:12.6
Point 4	0.5:1.5:1.0:0.8:12.2	0.5:1.6:2.2:2.2:15.1	0.5:1.6:0.6:1.4:12.9

parameters, the average crystallite size and the phases' percentage content derived from the XRD patterns. The original output files for all three samples (x = 0.8, 1, and 1.5) obtained by Topas 4.2 are given in the supplementary file.

Fig. 2 displays XRD-patterns in the 2-theta range 37.3° – 45.3° of $Ba_{0.5}Sr_{1.5}Zn_{1.2}Ni_{0.8}Fe_{12}O_{22}$, $Ba_{0.5}Sr_{1.5}ZnNiFe_{12}O_{22}$ and $Ba_{0.5}Sr_{1.5}Zn_{0.5}Ni_{1.5}Fe_{12}O_{22}$ treated at 1170 °C. No signs were observed of nickel spinel ferrite decomposition to NiO during the Y-type hexaferrite formation process [2].

The statistical data yielded by the analysis of the four points of EDX spectrum of polished cross-sections of the bulk samples of $Ba_{0.5}Sr_{1.5}Zn_{1.2}Ni_{0.8}Fe_{12}O_{22}$, $Ba_{0.5}Sr_{1.5}ZnNiFe_{12}O_{22}$ and $Ba_{0.5}Sr_{1.5}Zn_{0.5}Ni_{1.5}Fe_{12}O_{22}$ are given in Table 2.

2. Experimental design, materials, and methods

Polycrystalline samples of $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ (x = 0.8, 1, and 1.5) were fabricated by a modified citric acid sol-gel auto-combustion using stoichiometric amounts of the precursors; a detailed description of the sample preparation methodology is given in [1]. In brief, the powders produced after the auto-combustion process were annealed at 800 °C for three hours. All powders were subjected to homogenization by vibrating ball milling; then the resulting powders were pressed at 7 MPa to bulk pellets with a diameter of 16 mm. The pellets were heat-treated at 1170 °C in air for 10 h to obtain the $Ba_{0.5}Sr_{1.5}Zn_{2-x}Ni_xFe_{12}O_{22}$ compositions with $x = 0.8$, 1, and 1.5. Subsequently, the bulk pellets were cut and polished for microscopic studies.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2020.105803.

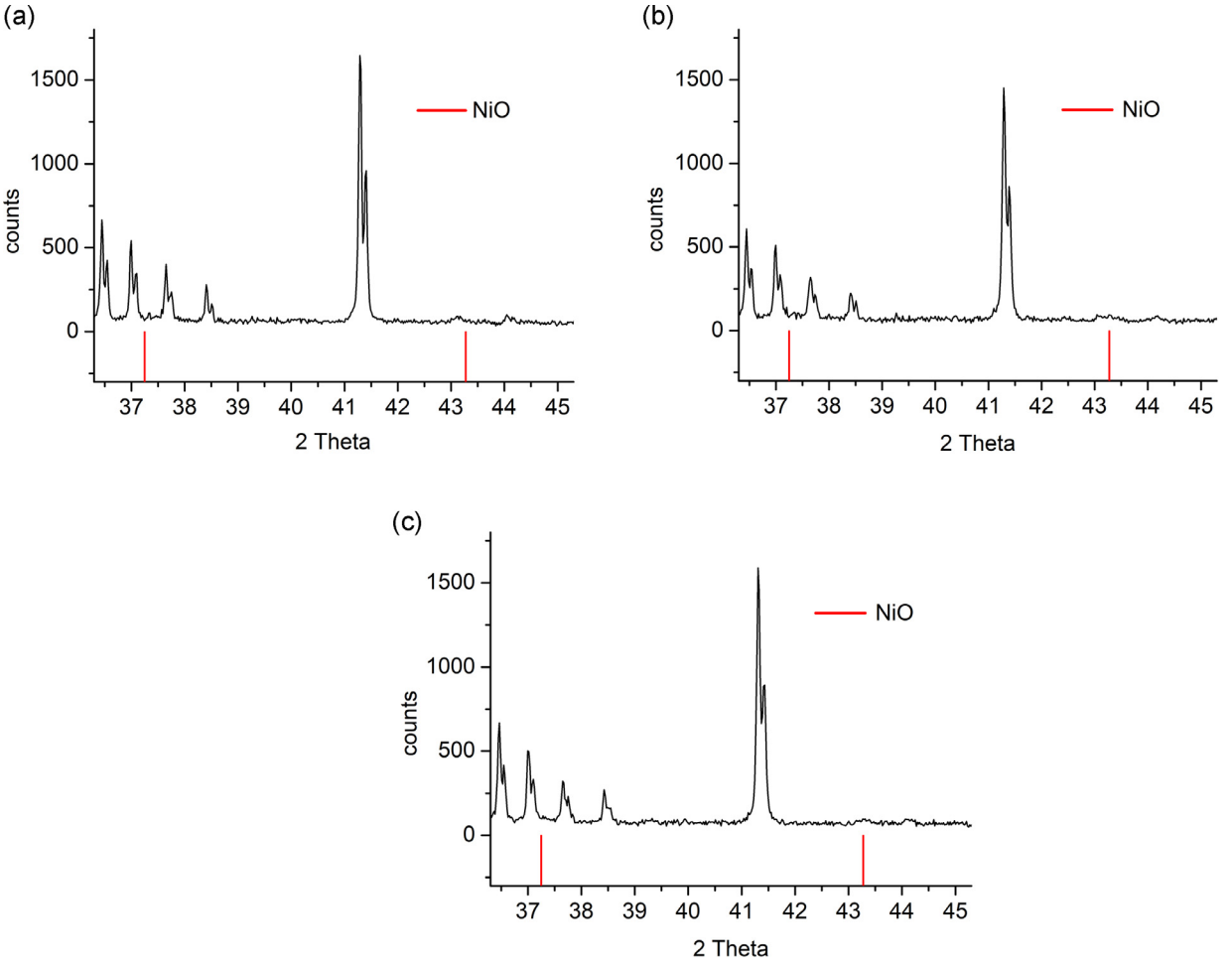

Fig. 2. XRD-patterns of (a) $Ba_{0.5}Sr_{1.5}Zn_{1.2}Ni_{0.8}Fe_{12}O_{22}$, (b) $Ba_{0.5}Sr_{1.5}ZnNiFe_{12}O_{22}$ and (c) $Ba_{0.5}Sr_{1.5}Zn_{0.5}Ni_{1.5}Fe_{12}O_{22}$ in the 2-theta range 37.3° – 45.3°. The expected peak positions of NiO (PDF number 00–047–1049) are marked in red.

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