Synchrotron X-ray Powder Diffraction Study of $Bi_2(Sr_{1-x}Eu_x)Ta_2O_9$ System

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A bismuth layered perovskite material $Bi_2SrTa_2O_9$ (BST), which consists of bismuth oxide layers and perovskite-like slabs, belongs to the family Aurivillius phases, are getting considerable attentions not only from ferroelectric thin film for application to ferroelectric random access memories (FeRAMs) but also from interlayer compounds for use to organic-inorganic hybrid composites. Recently, Ida and co-workers has been report the blue luminescent nanosheet derived from layered perovskite BST. The results give us new opportunities and challenges for search the new efficient luminescent materials having structures derived from the BST family. Thus, in this study a novel orange-red phosphor based on phosphate host crystal lattice, $Bi_2SrTa_2O_9$ doped with Eu^{3+} phosphors were synthesized by solid-state reaction using Bi_2O_3, $SrCO_3$, Ta_2O_5 and Eu_2O_3 as raw materials. The molar ratio of Bi : Sr : Ta : Eu was kept at 2 : 1-x : 2 : x, respectively. Stoichiometric homogeneous mixtures of highly pure raw materials were obtained by thorough grinding. The mixture was calcined in air at 1100°C for 6 hours. Synchrotron XRD patterns were taken with a large Debye-Scherrer camera installed at the BL01C2 beam line of NSRRC with λ = 0.5904 Å. The synchrotron XRD data were collected in a 2 θ range from 0.08° to 60° with a step interval of 0.02°. Structural refinements were made on X-ray diffractograms, by using the GSAS program.

Figure 1 shows experimental, calculated and difference in XRD patterns of $Bi_2Sr_{1-x}Ta_2O_9:Eu_x$ (x = 0.12) at room temperature (RT). An ideal crystal structure is also shown in the inset. All the observed peaks can be fitted with the reflection conditions in the monoclinic unit cell (space group: A 2_1 a m). The final structural parameters of $Bi_2Sr_{1-x}Ta_2O_9:Eu_x$ (x = 0, 0.04, 0.08 , 0.12 and 0.16) are summarized in Table 1. As seen from Table 1 and Fig. 2, Rietveld analysis afforded sufficiently low R (goodness of fit) factors. An decrease in lattice parameters and cell volume from x = 0 to x = 0.16 was observed, which is due to substitution of small size Eu^{3+} ions [1.066 Å for CN (coordination number) = 8] as compared to the smaller Sr^{2+} ions (1.26 Å for CN = 8).

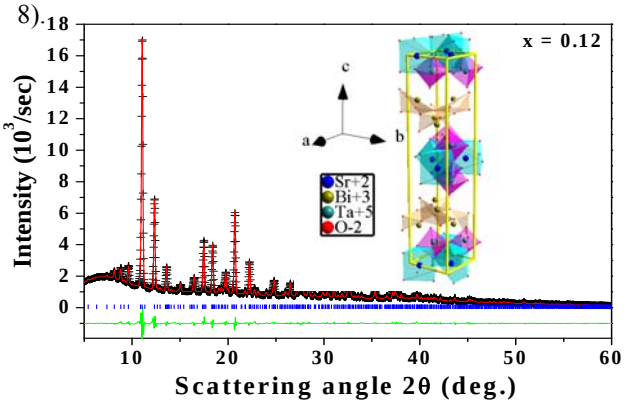

Fig. 1: Observed (crosses), calculated (solid line), and differences (bottom) synchrotron XRD pattern of $Bi_2Sr_{1-x}Ta_2O_9:Eu_x$ (x = 0.12) at RT with λ = 0.5904 Å. Bragg reflections are indicated by tick mark. An ideal crystal structure is also show in the inset.

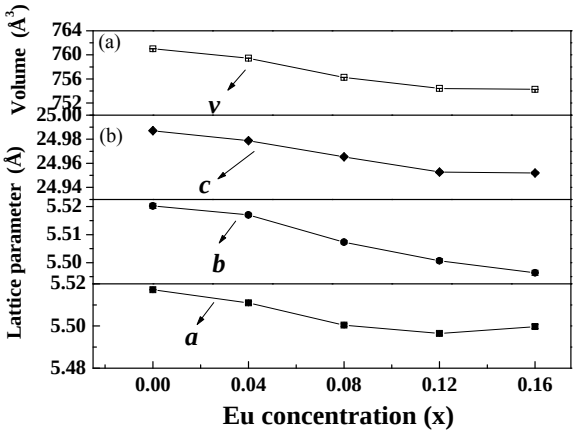

Fig. 2: The lattice parameters and unit cell volume are shown as a function of Eu concentration of $Bi_2Sr_{1-x}Ta_2O_9:Eu_x$ (x = 0, 0.04, 0.08 , 0.12 and 0.16). Error bars are smaller than symbol size.

Table 1: Refinement structure parameters of $Bi_2Sr_{1-x}Ta_2O_9:Eu_x$ (x = 0, 0.04, 0.08 , 0.12 and 0.16) at RT.

No.	x = 0	x = 0.04	x = 0.08	x = 0.12	x = 0.16
a/Å	5.5191(8)	5.5028(5)	5.4998(4)	5.4954(6)	5.4967(9)
b/Å	5.5198(8)	5.5103(5)	5.5080(4)	5.5019(6)	5.4992(9)
c/Å	24.9895(9)	24.9644(10)	24.9648(10)	24.9525(9)	24.9520(1)
V/ Å³	761.29(2)	756.98(1)	756.26(9)	754.44(1)	754.24(2)
Sr(Eu)					
x	-0.003(10)	-0.0035(17)	-0.0019(19)	-0.0091(15)	-0.010(5)
y	0.2527(31)	0.2672(20)	0.2673(22)	0.2634(21)	0.2637(25)
z	0	0	0	0	0
Uiso(Å²)	1.92(11)	1.43(8)	1.68(9)	1.55(8)	1.57(8)
Occupancy(Sr)	1	0.96	0.92	0.88	0.84
Occupancy(Eu)	0	0.04	0.08	0.12	0.16
Bi					
x	0.470(10)	0.475121	0.479685	0.478274	0.480(5)
y	0.7753(7)	0.7747(6)	0.7722(7)	0.7716(7)	0.7706(8)
z	0.20142(8)	0.20089(7)	0.20077(8)	0.20056(7)	0.20045(7)
Uiso(Å²)	4.02(7)	4.18(5)	4.21(6)	3.99(5)	3.92(5)
Ta					
x	0.512(10)	0.5118(7)	0.5144(8)	0.5115(7)	0.515(5)
y	0.7464(11)	0.7495(9)	0.7490(10)	0.7499(10)	0.7512(12)
z	0.41435(6)	0.41457(5)	0.41480(6)	0.41488(5)	0.41515(5)
Uiso(Å²)	1.386(29)	1.465(21)	1.478(23)	1.535(22)	1.548(23)
O(1)					
x	0.471(20)	0.533(24)	0.797(68)	1.118(80)	0.95032
y	0.157(11)	0.245(23)	0.329(37)	0.439(84)	1.1923
z	0	0	0	0	0
Uiso(Å²)	2.50	18.9(24)	80.0(25)	80.0(22)	80.0(15)
O(2)					
x	0.525(13)	0.513(9)	0.522(11)	0.547(6)	0.55506
y	0.672(13)	0.700(5)	0.696(8)	0.724(8)	0.74133
z	0.3481(10)	0.3387(7)	0.3378(10)	0.3355(7)	0.32949
Uiso(Å²)	2.50	1.6(6)	2.50	0.8(6)	2.0(7)
O(3)					
x	0.73810	0.736(9)	0.731(10)	0.749(12)	0.745(16)
y	0.99230	1.009(21)	1.028(11)	0.983(19)	0.968(24)
z	0.25076	0.2395(9)	0.2322(13)	0.2373(10)	0.2348(13)
Uiso(Å²)	1.2(6)	0.2(5)	2.50	3.1(9)	6.4(13)
O(4)					
x	0.800(14)	0.811(9)	0.810(10)	0.788(14)	0.773(13)
y	1.079(12)	1.044(12)	1.101(11)	1.031(13)	1.051(13)
z	0.0659(19)	0.0618(15)	0.0589(19)	0.0614(25)	0.0723(24)
Uiso(Å²)	3.8(14)	4.6(13)	5.9(15)	4.1(11)	2.50
O(5)					
x	0.763(14)	0.757(14)	0.785(16)	0.745(15)	0.760(17)
Y	1.013(10)	0.992(12)	1.029(16)	1.022(15)	0.968(17)
z	0.5742(17)	0.5795(12)	0.5754(14)	0.5764(19)	0.5689(24)
Uiso(Å²)	2.50	2.50	2.50	2.50	2.50
Rp%/Rwp%	2.48/3.69	2.35/3.38	2.86/4.02	2.50/3.69	2.52/3.67
χ^2	1.29	1.03	1.69	1.24	1.141