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Studies on X – doped (X = Al, Zn and Cu) and undoped Lead Iodide single crystals relating to XRD

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ABSTRACT

X – doped (X = Al, Zn and Cu) and undoped Lead Iodide crystals were grown by gel technique by single diffusion method. After the complete growth of X – doped and undoped Lead Iodide crystals in test tube, they were taken out carefully from the test tube.Then, they are washed with acetone and dried for whole night under light. Then, they are crushed in a size of 150 mesh. As-grown crystals were subjected to XRD, lattice parameters, hkl plane and structure compared and reported.

Keywords: Gel technique, XRD.

INTRODUCTION

Band gap of Lead Iodide crystals is about 2.55 eV having layered structure similar to Cadmium Iodide, atoms are located in layers of Pb and I perpendicular to c-axis in the succession I-Pb-I-I-Pb-I. Compounds exhibiting a structure of this kind possess a strong intralayer bonding, ionic in nature. Whereas Lead Iodide is highly insulating material with a resistivity of about 10^{12} ohm-cm. Variours properties has been studied by different researchers.

In the present course of investigation it has been decided, on the preliminary view, to study on X – doped and undoped Lead Iodide single crystals especially on XRD.

MATERIALS AND METHODS

X - doped (X = Al, Zn and Cu) and undoped Lead Iodide single crystals have been synthesized by gel method. A.R.grade chemicals were used throughout the work. Acetic Acid (5 ml) was taken in the beaker, drop by drop, Sodium Metasilicate added with constant stirring by magnetic stirrer till 4 pH obtained. Then Lead Acetate and Aluminium Chloride (5 ml each) added in the

above mixture with constant stirring. These mixtures poured in the test tube. The mouth of the test tube covered by cotton. After 10 to 12 days gel get set. Then, Potassium Acetate poured slowly over the set gel. After 10 days crystals were takent out from the test tube. These crystals are crushed in a uniform size (150 mesh). The Xray diffraction patterns of the deposited films were recorded with the help of X-ray diffractometer (Philips PW XL-1730) using CuKα radiation Ni filter (1.5418 Å). The XRD patterns of all the films were taken from 20 to 90^0 (2θ). The peaks of the patterns were searched by computer programming method. Similar procedure were adopted for Zn and Cu doping.

RESULTS AND DISCUSSION

X-ray diffraction

X-ray diffractometry is useful in analyzing crystal structure, evaluation of 'd' values, cell parameters, system to which the sample under study belongs, grain size, microstrain, reflecting planes etc. Records of X-ray powder diffraction patterns of these samples, doped and undoped Lead Iodide crystals, under identical conditions signifies that the samples belongs to hexagonal system and are crystalline in nature. Fig. 1, 2, 3, and 4 represents an X-ray diffractogram of undoped and X-doped (X= Al, Zn and Cu) respectively. Similar X-ray diffractogram were obtained for undoped Lead Iodide crystals [1]. The observed and calculated 'd' values are given Table 1. 2, 3 and 4 for undoped and X-doped (X= Al, Zn and Cu) Lead Iodide crystals respectively.

The lattice parameters 'a' and 'c' of all the samples are well matching with the ASTM data of Lead Iodide. It may be seen from this table that the unit cell volume is sensitively affected by dopant concentrations. Similar results were given for CdS [3]. As seen from Fig.3, the height of peaks goes on increasing as the dopant concentrations increases for Cu-doped Lead Iodide crystals while Fig. 2 and Fig. 3 depicts the height of peaks decreases as the dopant concentrations increases for Al-doped and Zn doped Lead Iodide crystals respectively.

Explanation of doping

Effect of dopant concentration on lattice parameters may be explained as follows (i) Al-doped in the form of Al-acetate presumably dissociates into aluminium ion and acetate ion. Aluminium ion (ionic radius=0.5 Å) might be replacing lead ion maintaining the charge neutrality. As the radii of the substituted ions are shorter than the replacing ions, the lattice parameters and the unit cell volume remain unaltered at lower concentration in the lead iodide crystals, (ii) at higher Al dopant concentration (above 0.1M), the non-isoelectronic substitution may results in the creation of cation vacancies. The substitution of aluminium ions at cation site leads to the creation of cation vacancies. The vacancies so created in the lattice might be responsible for the increase in the values of unit cell volume and (iii) as the lead iodide crystals are layered structures, the doping affects more in 'c' lattice parameter than 'a' lattice parameter as seen in the Table 2.

Similar arguments may apply to Cu-doped and Zn-doped Lead Iodide crystals

Table 1 X-ray powder diffraction data (Lead Iodide crystals).

'd' values		I/I_o	hkl plane
diffractogram	computer		

3.5036	3.5269	92	0 0 2
2.6496	2.6297	66	1 0 2
2.3540	2.3512	65	0 0 3
2.0299	2.0199	54	1 0 3
1.9163	1.9138	30	1 1 2
1.7634	1.7634	100	0 0 4
1.7323	1.7220	33	2 0 2
1.6407	1.6363	33	1 1 3
1.6040	1.6100	26	1 0 .4
1.4700	1.4594	29	2 1 1
1.3955	1.3946	46	1 1 4
1.3774	1.3738	28	2 1 2
1.3232	1.3284	80	3 0 0
1.2624	1.2595	26	2 1 3

Table 2 X-ray powder diffraction data (Al-doped Lead Iodide crystals)

'd' values						I/I_o			hkl plane		
diffracto.	computer	diffracto.	computer	diffracted.	computer	0.1 Al	0.5 Al	1Al	0.1 Al	0.5 Al	1Al
3.5588	3.5395	3.5310	3.5310	3.5588	3.5395	24	51	92	0 0 2	0 0 2	0 0 2
2.6804	2.6350	2.6694	2.6315	2.6804	2.6350	33	61	100	1 0 2	1 0 2	1 0 2
2.3779	2.3597	2.3659	2.3540	2.3779	2.3597	82	93	66	0 0 3	0 0 3	0 0 3
2.0386	2.0253	2.0299	2.0217	2.0386	2.0253	31	35	63	1 0 3	1 0 3	1 0 3
1.7698	1.7698	1.7634	1.7655	1.7698	1.7698	100	43	81	0 0 4	0 0 4	0 0 4
1.6515	1.6391	1.3955	1.3956	1.3992	1.3977	17	100	63	1 1 3	1 1 4	1 1 3
1.3992	1.3977	1.1210	1.1247	1.3264	1.3326	24	37	68	1 1 4	2 2 1	3 1 0
1.3264	1.3326					32			1 0 5		
1.1231	1.1248					23			2 2 1		
1.1190	1.0946					22			3 1 0		

Table 3 X-ray powder diffraction data (Zn-doped Lead Iodide crystals)

'd' values						I/I_o			hkl plane		
diffracto.	computer	diffracto.	computer	diffracto.	computer	0.1 Zn	0.5 Zn	1 Zn	0.1 Zn	0.5 Zn	1 Zn
3.4502	3.4514	3.5588	3.5524	3.5310	3.5310	09	18	24	1 0 1	0 0 2	0 0 2
2.6496	2.6292	2.6961	2.6449	2.6649	2.6361	24	31	26	1 0 2	1 0 2	1 0 2
2.3540	2.3528	2.3901	2.3682	2.3659	2.3540	79	62	74	0 0 3	0 0 3	0 0 3
2.2962	2.2875	2.0473	2.0328	2.0299	2.0238	18	29	18	1 1 0	1 0 3	1 0 3
2.1892	2.1752	1.7762	1.7762	1.9163	1.9198	09	43	13	1 1 1	0 0 4	1 1 2
2.0213	2.0166	1.4030	1.4029	1.7634	1.7655	18	100	100	1 0 3	1 1 4	0 0 4
1.9087	1.9067	1.3279	1.3225	1.7323	1.7277	10	33	14	2 0 1	2 0 4	2 0 2
1.7571	1.7571			1.6407	1.6405	100		15	0 0 4		1 1 3
1.5131	1.5127			1.3955	1.3976	10		22	2 0 3		1 1 4
1.4617	1.4646			1.3810	1.3787	11		15	2 1 1		2 1 2
1.3919	1.3935			1.3297	1.3304	19		15	1 1 4		3 0 0
1.3774	1.3777			1.3232	1.3304			26	2 1 2		1 0 5
1.3200	1.3208								3 0 0		

Table 4 X-ray powder diffraction data (Cu-doped Lead Iodide crystals).

'd' values						I/I_o			hkl plane		
diffracto.	computer	diffracto.	computer	diffracto.	computer	0.1Cu	0.5Cu	1Cu	0.1Cu	0.5Cu	1Cu
3.5036	3.5269	3.5588	3.5524	3.5036	3.5269	73	32	92	0 0 2	0 0 2	0 0 2
2.6496	2.6407	2.6804	2.6513	2.6496	2.6297	82	49	66	1 0 2	1 0 2	1 0 2
2.3540	2.3512	2.3779	2.3682	2.3540	2.3512	83	90	65	0 0 3	0 0 3	0 0 3
2.0299	2.0249	2.0473	2.0357	2.0299	2.0199	61	32	54	1 0 3	1 0 3	1 0 3
1.7634	1.7634	1.7698	1.7762	1.9163	1.9138	100	100	30	0 0 4	0 0 4	1 1 2
1.3919	1.3946	1.3992	1.3863	1.7634	1.7634	58	21	100	1 1 4	1 0 5	0 0 4
1.3232	1.3284	1.3297	1.3297	1.7323	1.7220	77	36	33	3 0 0	3 0 0	2 0 2
				1.6407	1.6363			33			1 1 3
				1.6040	1.6100			26			1 0 4
				1.4700	1.4594			29			2 1 1
				1.3955	1.3946			46			1 1 4
				1.3774	1.3738			28			2 1 2
				1.3232	1.3284			80			3 0 0
				1.2624	1.2595			26			2 1 3

Table 5 Effect of preparative conditionons lattice parameters

Compound	dopant concentration (molar)	Lattice parameters a (Å)	c (Å)	c/a	$V(Å)^3$
Reported	-	4.575	6.989	1.5277	126.69
Undoped	-	4.575	7.0357	1.5379	127.53
Al-doped	0.1	4.575	7.079	1.5473	128.32
Al-doped	0.5	4.575	7.062	1.5436	128.01
Al-doped	1.0	4.575	7.079	1.5473	128.32
Zn-doped	0.1	4.575	7.0285	1.5363	127.40
Zn-doped	0.1	4.575	7.1047	1.5529	128.78
Zn-doped	0.1	4.575	7.062	1.5436	128.01
Cu-doped	0.1	4.575	7.0545	1.5420	127.87
Cu-doped	0.1	4.575	7.1047	1.5529	128.78
Cu-doped	0.1	4.575	7.0537	1.5418	127.86

Intensity in cps

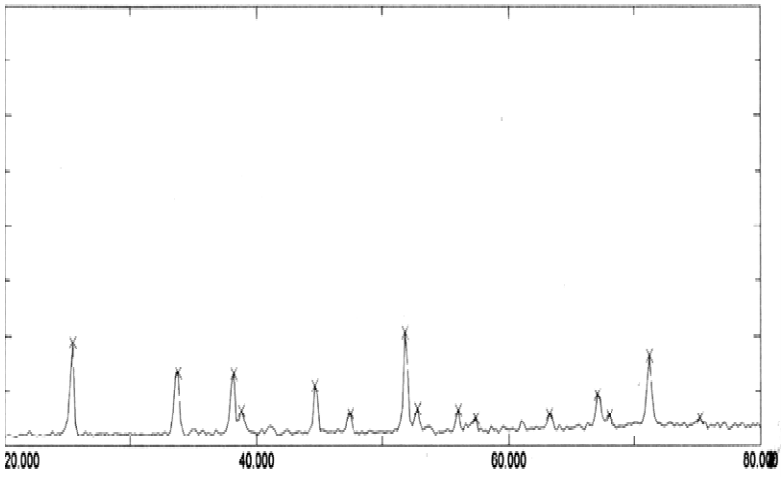

Fig. 1 X-ray diffractogram for undoped Lead Iodide crystals Intensity in cps

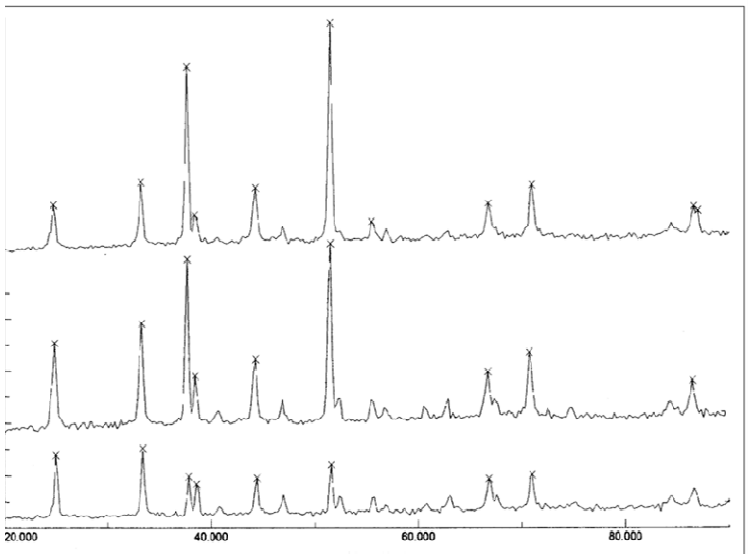

Fig. 2 X-ray diffractogram for Al-doped Lead Iodide crystals (from top 0.1, 0.5 and 1 Molar concentration)

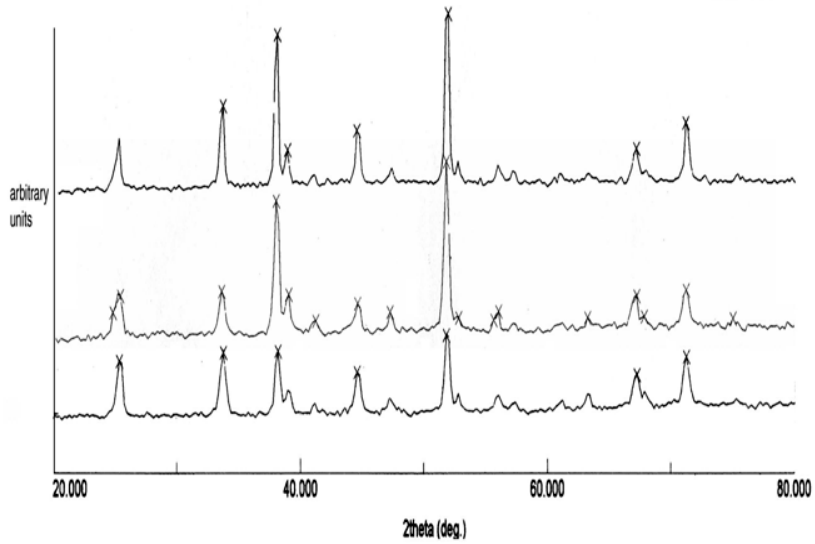

Fig. 3 X-ray diffractogram for Zn-doped Lead Iodide crystals (from top 0.1, 0.5 and 1 Molar concentration)

Intensity in cps

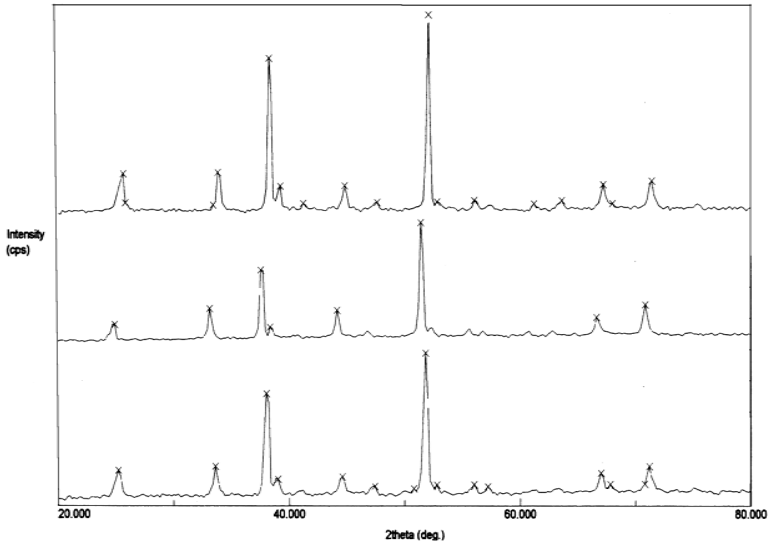

Fig. 4 X-ray diffractogram for Cu-doped Lead Iodide crystals (from bottmm 0.1, 0.5 and 1 Molar concentration)

CONCLUSION

1) Lattice constants ‘a’ and ‘c’ and hence the unit cell volume are sensitively affected by the dopant concentrations
2) Unit cell volume tends to increase with dopant concentrations
3) There is no dilation of the unit cell along ‘a’ or ‘c’ direction as the ratio of ‘c/a’ is almost constant.

4) The addition of $CuCl_2$ into PbI_2 in the present case is considered to enhance the atomic rearrangement by creation of Pb vacancies.

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