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Comparative studies on XRD and band gap of thin films of gel grown, doped and undoped PbI_2, and pure powder of PbI_2

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ABSTRACT

Lead Iodide single crystals successfully grown by simple gel method. Some dopants were added into the Lead Iodide crystals with proper precaution. Thin films of pure material of Lead Iodide and gel grown crystals have been prepared by thermal evaporation technique. XRD of these films were recorded and compared. Lattice parameters have been calculated by computer programming and they are matching with the JCPDS data of the Lead Iodide XRD of all the films are compared and reported. Lattice constants are observed to be sensitively affected by doping. The band gaps of these films were calculated by measuring the transmittance. It is found that the energy band gap of these films goes on decreasing as the thickness of the films increased. The band gaps of the doped films were found to decrease significantly.

Keywords: Gel Technique, Thin Films, XRD, Band Gap.

INTRODUCTION

Lead Iodide (PbI2), IV-VII semiconducting compound with a band-gap of approximately 2.55 eV at room temperature, has a layered structure of different polytypes that are generally hexagonal in shape. It is a highly insulating material with a resistivity of about 1012 ohm-cm.The high atomic numbers of Pb and I (Z= 82 and 53, respectively) yield superior stopping power for high energy x-rays and gamma-rays [1]. Compact room-temperature x-ray and gamma-ray detectors with improved energy resolution have an enormous range of medical, industrial, military, space, and environmental applications. The requirement for room temperature operation in many applications requires use of a material with a higher atomic number for increased stopping power and larger band-gap for reduced dark current. Presently, Hg12 and CdTe are the most frequently used materials for fabricating room temperature radiation detectors [2].

This material has been the subject of many investigations due to specific technological features, for instance, its large applicability, at room temperature, as photocell, and x- and γ-ray detector (3). Lead Iodide is more attractive than other similar materials, such as HgI_2, because of its lower vapour pressure and lack of a destructive phase transition, which shows up at temperature around

130^0C for Hg_2. The electronic structure and optical properties were studied both experimentally and theoretically (3).

Although studies of bulk crystals are essential for understanding some of the fundamental properties of the material, the preparation and study of high quality thin films are desirable for device applications. In the present course of investigation, it has been decided, on the preliminary basis, to compare the XRD and the band gap of the doped, pure and synthesized Lead Iodide crystals and thin films. In the course of present investigation, we have observed that: (i) the lattice parameters 'a' and 'c' and hence the unit cell volume of doped, pure and synthesized Lead Iodide crystals, are sensitively affected by the dopant concentration and thickness of the films. (ii) band gap of the undoped Lead Iodide films matches with the reported value (iii) band gap of doped Lead Iodide films were decreases significantlly. The purpose of this communication is to find out the influence of doping regarding the band gap to prepare the photovoltaic application in the future.

MATERIALS AND METHODS

The doped (Cu and Al with different concentrations) and undoped Lead Iodide crystals have been grown by gel technique. These crystals were crushed in standard size (150 mash). The A.R. grade chemicals were used for this purpose. Then the thin films of (i) as grown Lead Iodide crystals, doped and undoped, and (ii) of pure Lead Iodide material, were prepared by vacuum technique. The evaporation is carried out in a conventional vacuum coating unit of 10^{-5} torr, with constant substrate temperature of 80^0C. The thickness was measured by quartz crystal thickness monitor make by HindHivac DTM model no.101. Care must be taken to avoid overheating the stock of Lead Iodide during sublimation, otherwise thermal decomposition gives rise to non-stoichiometry in the films, apart from this no special precaution are necessary.

X-ray diffractograms of all these films were recorded with Philips X-ray diffractometer (Model PW-1730) using CuKα with Ni filter (1.5418Å). Transmissions of these films were recorded using Hitachi-331.

RESULTS AND DISCUSSION

The diffractometer recordings for thin films grown at 300K on glass substrate of pure and synthesized Lead Iodide material (doped and undoped) with various thicknessess are shown in Fig. 1, Fig. 2, Fig. 3, Fig. 4, Fig. 5 and Fig. 6 for comparison. Where as diffractometer recording for synthesized and pure Lead Iodide material shows a sharp peak is at 2θ=25.400, 36.600 and 52.200. The common sharp peak is at 52.200 only, corresponding to (0 0 4) lattice plane. Fig.1 clearly indicates that as the thickness of the film, synthesized undoped Lead Iodide, increases the height of the peak increases also Fig. 2 and Fig. 3 shows that the height of the peak increases sharply with increase in thickness for pure Lead Iodide material. Similarly Fig.4 and Fig. 5 represents that the peaks of Cu-doped films increases sharply with increase in thickness while Fig. 6 depicts the height of peaks of Al-doped films decreases with increasing thickness. The intensity of Cu-doped films is very large as compared to all the other films.

The lattice parameters 'a' and 'c' of these films have been computed from the observed'd' values by method of successive refinement. Mean values of lattice parameters are given in Table 1. It may be seen from this table that lattice constants 'a' and 'c' and hence the unit cell volume is sensitively affected by doping.

Table 2 shows the transmission data of all the films in uv-visible range. The values of the magnitude of optical absorption coefficient are of the order of 10^5 cm^{-1} for near edge absorption given by α=lnT/t where, t is the thickness of the film. The values of α have been calculated, at different wavelengths, from Table 2. The plots of $(\alpha h\nu)^2$ versus hν(given in Figure 7 to 14), from which the band gaps are calculated and represented in Table 3, are given for comparision. This is due to allowed direct transition from the top of valence band to the conduction band minimum at the center of Brillouin zone [4].

From Table 3 it is clearly seen that the variation in thickness causes a slight decrease in direct allowed optical band gap Eg. Further, it can also be seen from Table 2 that the band gap for Cu-doped film decreases significantly. This is due to the fact that the excess Cu ion in the lattice makes the donar levels degenerate and merges into the conduction band of Cu-doped films thus decreasing the optical band gaps.

The absorption coefficient α also changes with thickness, particularly in Cu-doped films. It is therefore suggested that Cu-doped films will be of use in photovoltaic device applications.

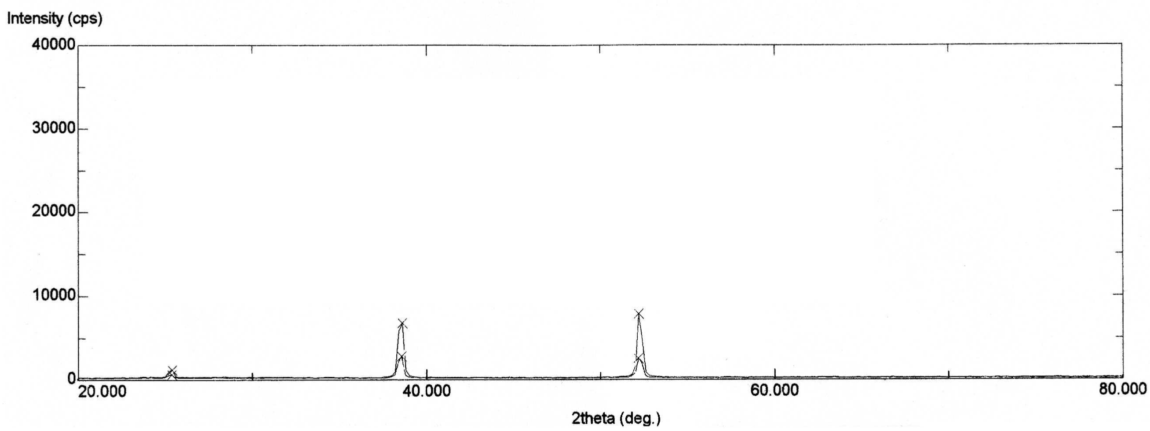

Fig. 1 X-ray diffractogram of synthesized PbI2 films (1000 and 2000 Å)

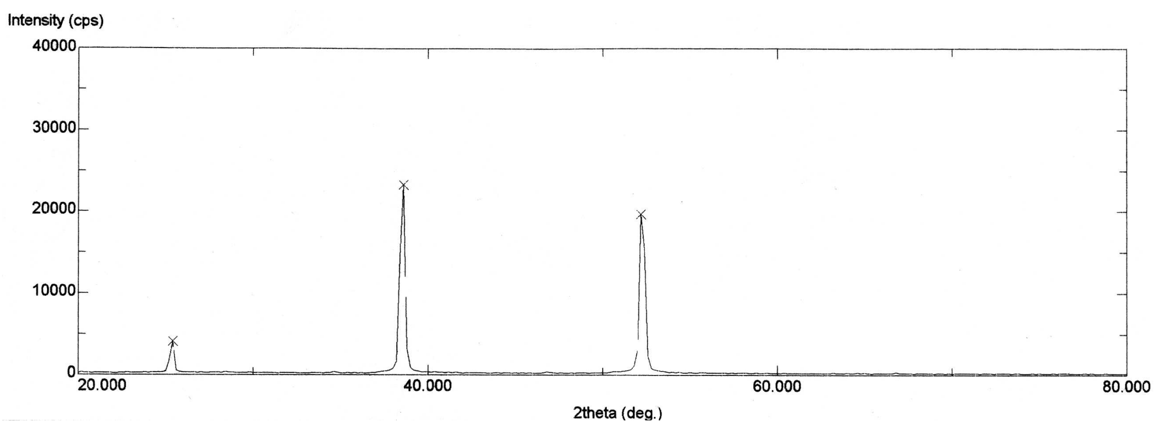

Fig. 2 X-ray diffractogram of pure PbI2 films (1000 Å)

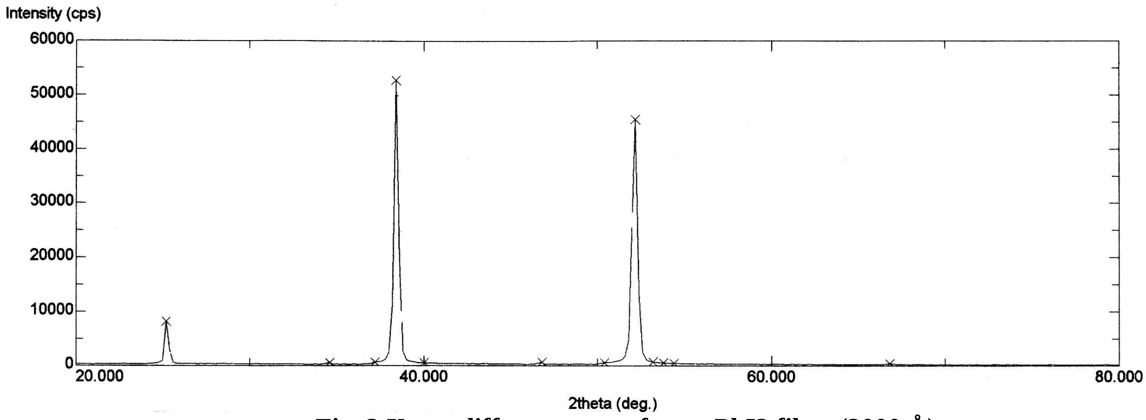

Fig. 3 X-ray diffractogram of pure PbI2 films (2000 Å)

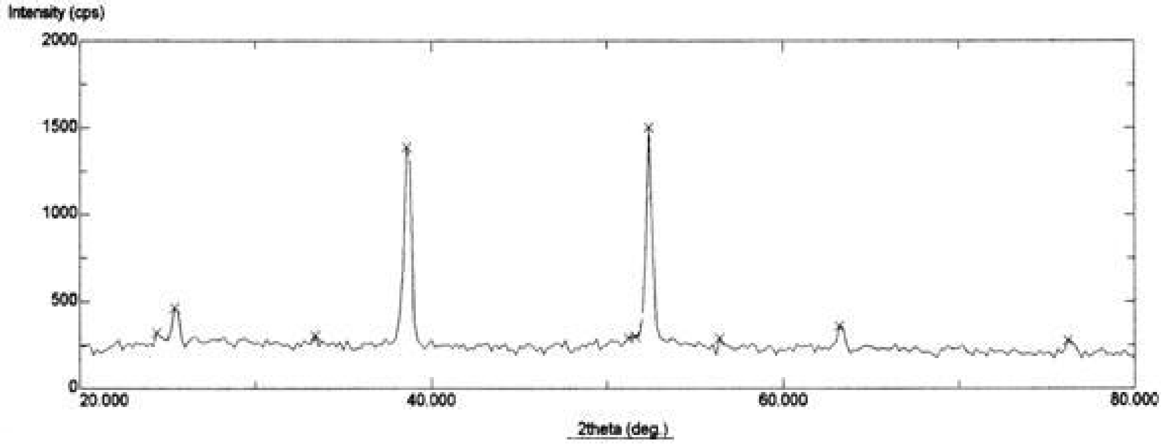

Fig. 4 X-ray diffractogram of Cu-PbI2 films (2000 Å)

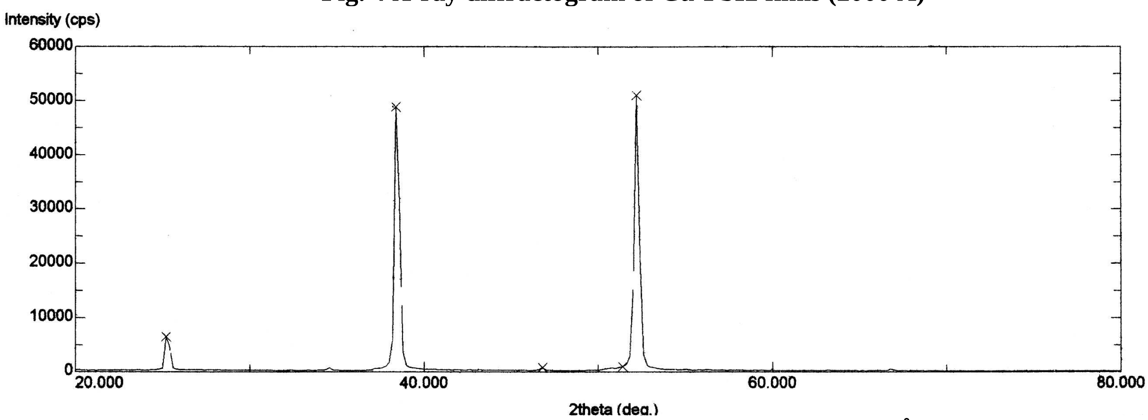

Fig. 5 X-ray diffractogram of Cu-PbI2 films (4000 Å)

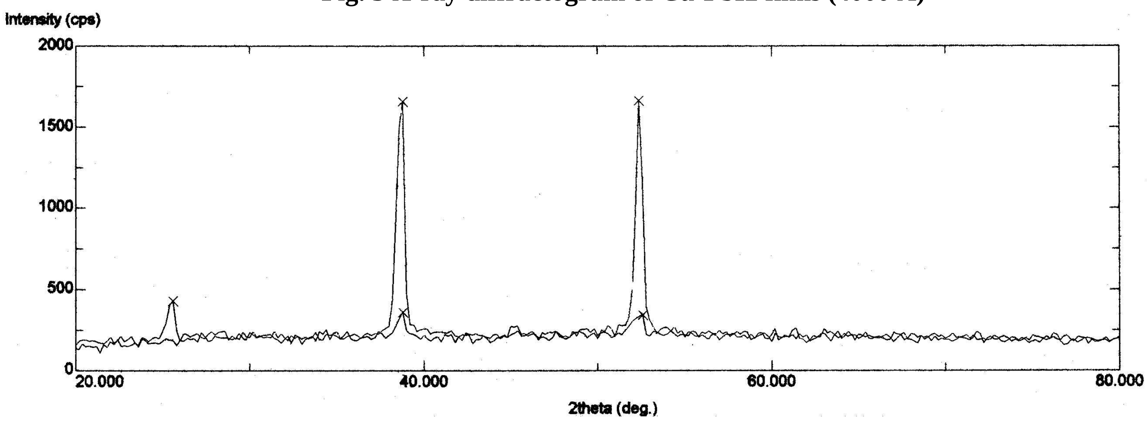

Fig. 6 X-ray diffractogram of Al-PbI2 films (2000 and 4000 Å)

Table 1: Comparative study of XRD with lattice parameters.

Compound	Thickness in Å	Lattice Parameters 'a' in Å	'c' in Å	c/a	V ($Å^3$)
i) synthesized un-doped film	1000	4.557	7.01	1.5383	126.93
	2000	4.557	7.01	1.5383	126.93
ii) pure undoped film	1000	4.557	7.01	1.5383	126.93
	2000	4.557	7.0264	1.5419	126.36
iii) Cu-doped film	2000	4.557	6.9785	1.5314	125.5
	4000	4.557	7.003	1.5368	125.94
iv) Al-doped film	2000	4.6	7.2299	1.5717	132.45
	4000	4.612	7.2301	1.5676	133.18

Table 2

Wavelength In µ	Transmission for Synth. Cry. Films		Pure Material Films		Cu-doped Films		Al-doped Films	
	1000Å	2000Å	1000Å	2000Å	2000Å	4000Å	2000Å	4000Å
0.70	0.559	0.397	0.550	0.604	0.537	0.422	0.478	0.263
0.68	0.520	0.375	0.587	0.540	0.483	0.374	0.433	0.243
0.66	0.480	0.355	0.614	0.463	0.447	0.394	0.432	0.252
0.64	0.441	0.341	0.612	0.413	0.437	0.486	0.489	0.256
0.62	0.407	0.335	0.569	0.415	0.464	0.510	0.589	0.217
0.60	0.376	0.334	0.498	0.485	0.532	0.379	0.562	0.194
0.58	0.360	0.350	0.426	0.540	0.616	0.337	0.427	0.207
0.56	0.362	0.373	0.378	0.430	0.566	0.456	0.374	0.164
0.54	0.394	0.370	0.385	0.341	0.399	0.321	0.496	0.160
0.52	0.453	0.266	0.433	0.403	0.348	0.349	0.305	0.105
0.50	0.087	0.047	0.043	0.090	0.027	0.001	0.007	
0.48	0.066	0.035	0.030	0.040	0.017		0.003	
0.46	0.030	0.015	0.010		0.004			
0.44	0.008	0.002	0.001					
0.42	0.001							

Table :3 Comparative study of band gap

Compound	Thickness in Å	Band Gap in eV
i) synthesized undoped film	1000	2.623
	2000	2.5802
ii) pure undoped film	1000	2.5255
	2000	2.3497
iii) Cu-doped film	2000	2.464
	4000	2.295
iv) Al-doped film	2000	2.454
	4000	2.359

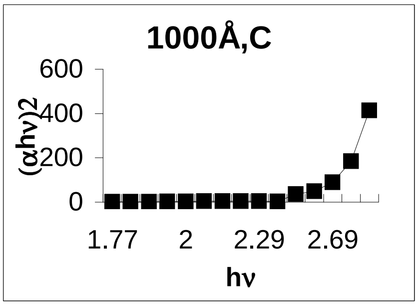

Fig. 7

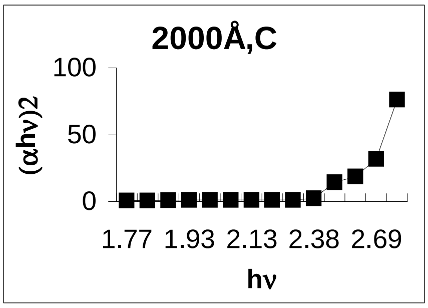

Fig. 8

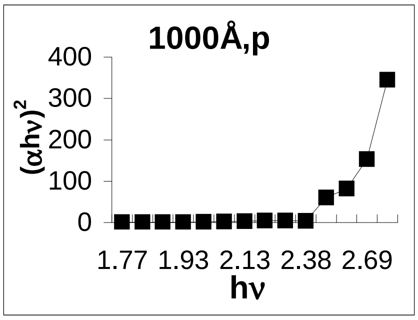

Fig. 9

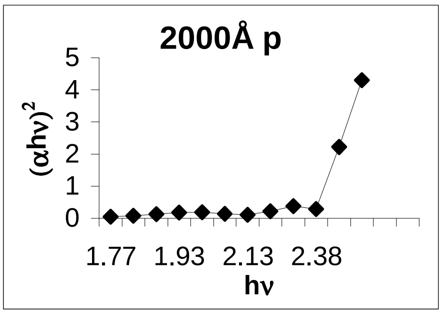

Fig. 10

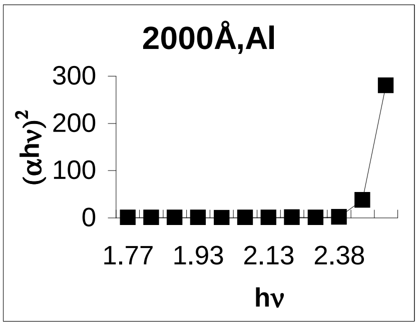

Fig. 11

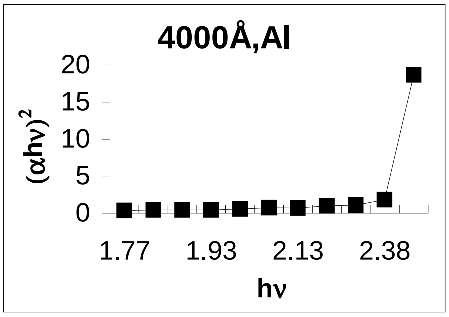

Fig. 12

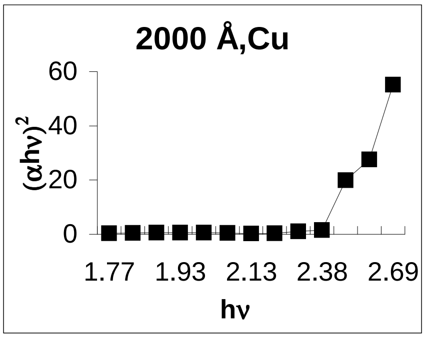

Fig. 13

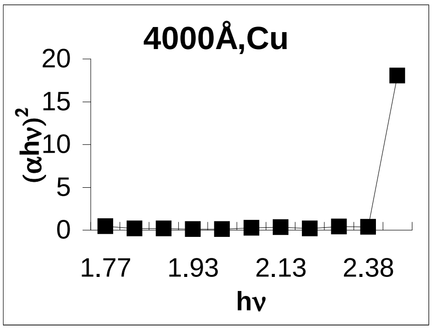

Fig. 14

CONCLUSION

i) With proper doping in the Lead Iodide, either Cu or Al, leads to significant decrease in the band gap.
ii) This doped films may be used as a photovoltaic cell
iii) Lattice constants 'a' and 'c' and the unit cell volume are sensitively affected by the doping.

iv) Unit cell volume tends to increase with increase in the thickness of the films particularly in case of doped films.

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