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Influence of Doping on Lead Iodide Crystals

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ABSTRACT

The undoped and doped Lead Iodide crystals have been grown by gel technique at room temperature. The thin films of these gel grown crystals have been grown on a glass substrate by vacuum technique. XRD of these films were recorded and compared. They are almost matching with ASTM data of Lead Iodide. 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, band gap.

INTRODUCTION

Lead iodide, PbI_2, is a direct band gap p-type semiconductor with a layered structure. The atomic arrangement is in the form of layers of Lead and Iodine atoms oriented perpendicularly to the c-axis. They consists of molecular sheets, each consisting of a layer of cation sandwiched between two layers of hexagonal close packed anion. The forces within the sandwiched are purely ionic in nature, giving a strong binding between an anion and cation layer, whereas the anion layer in adjacent sandwiches are held together by weak van der Wall's forces of attraction. The layers can be stacked in a variety of ways to form different types of polyptism.

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 [1-6]. 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 [1,2,5,7-9]. The electronic structure and optical properties were studied both experimentally [10-14] and theoretically [15-17].

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. With an aim to investigate the effect of doping on optical properties of Lead

Iodide, work on preparation and characterization of pure and synthesized doped and undoped Lead Iodide thin films in polycrystalline form has been undertaken.

In the course of present investigation, we have observed that: (i) the lattice parameters ‘a’ and ‘c’ and hence the unit cell volume are sensitively affected by the dopant concentration. (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 present effect of doping on the band gap of Lead Iodide films.

MATERIALS AND METHODS

The doped 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, thin films of these gel grown Lead Iodide crystals 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 gel grown undoped Lead Iodide and Al-doped thin films of gel grown Lead Iodide at 300K on glass substrate with various thicknessesses are shown in Fig. 1 and 2 respectively. Diffractometer recording for the thin films of different thickness shows a sharp peak is at 2θ=25.40, 36.60 and 52.20^0. The common sharp peak is at 52.20^0 only, corresponding to (0 0 4) lattice plane. Fig.2 clearly indicates that as the thickness of doped thin films increases, the height of the peak increases, also the height of the peak increases sharply.

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 $h\nu$ (given in Fig, 3 to 6), 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 (18).

From Table 3 it is clearly seen that the variation in thickness causes a slight decrease in direct allowed optical band gap Eg. This is due to the fact that the excess Al ion in the lattice makes the donar levels degenerate and merges into the conduction band of Al-doped films thus decreasing the optical band gaps.

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

Table 1

Compound	Thickness in Å	Lattice Parameters 'a' in Å	'c' in Å	c/a	V (Å^3)
i) Gel grown PbI2	----	4.618	7.11	1.5465	127.23
ii) Thin films of undoped PbI_2 (Not shown)	1000	4.557	7.01	1.5383	126.93
	2000	4.557	7.01	1.5383	126.93
iii) Thin films Al-doped PbI_2	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 Undoped PbI_2 Films 1000Å	2000Å	Al-doped Films 2000Å	4000Å
0.70	0.559	0.397	0.478	0.263
0.68	0.520	0.375	0.433	0.243
0.66	0.480	0.355	0.432	0.252
0.64	0.441	0.341	0.489	0.256
0.62	0.407	0.335	0.589	0.217
0.60	0.376	0.334	0.562	0.194
0.58	0.360	0.350	0.427	0.207
0.56	0.362	0.373	0.374	0.164
0.54	0.394	0.370	0.496	0.160
0.52	0.453	0.266	0.305	0.105
0.50	0.087	0.047	0.001	0.007
0.48	0.066	0.035		
0.44	0.030	0.015		
0.45	0.008	0.002		
0.46	0.42	0.001		

Table 3

Compound	Thickness in Å	Band Gap in eV
i) Undoped thin films of PbI2	1000	2.623
	2000	2.5802
iv) Al-doped film	2000	2.454
	4000	2.359

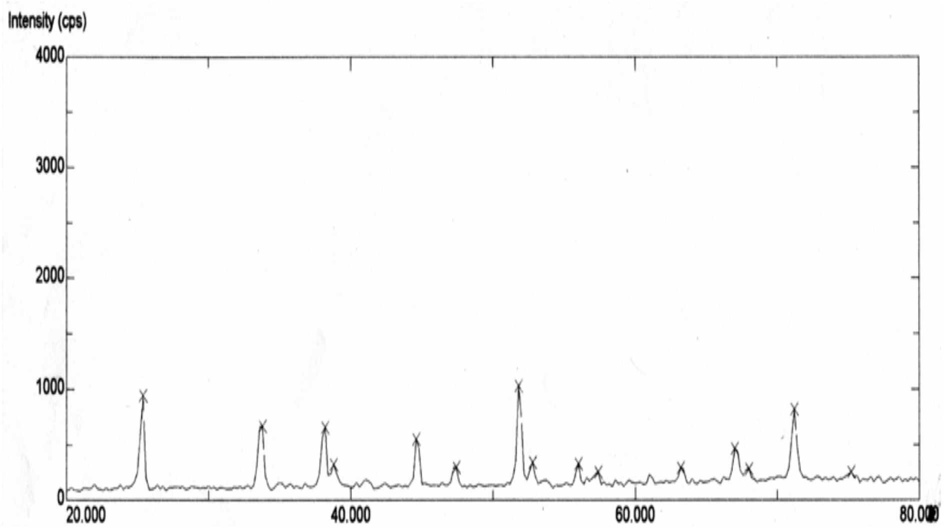
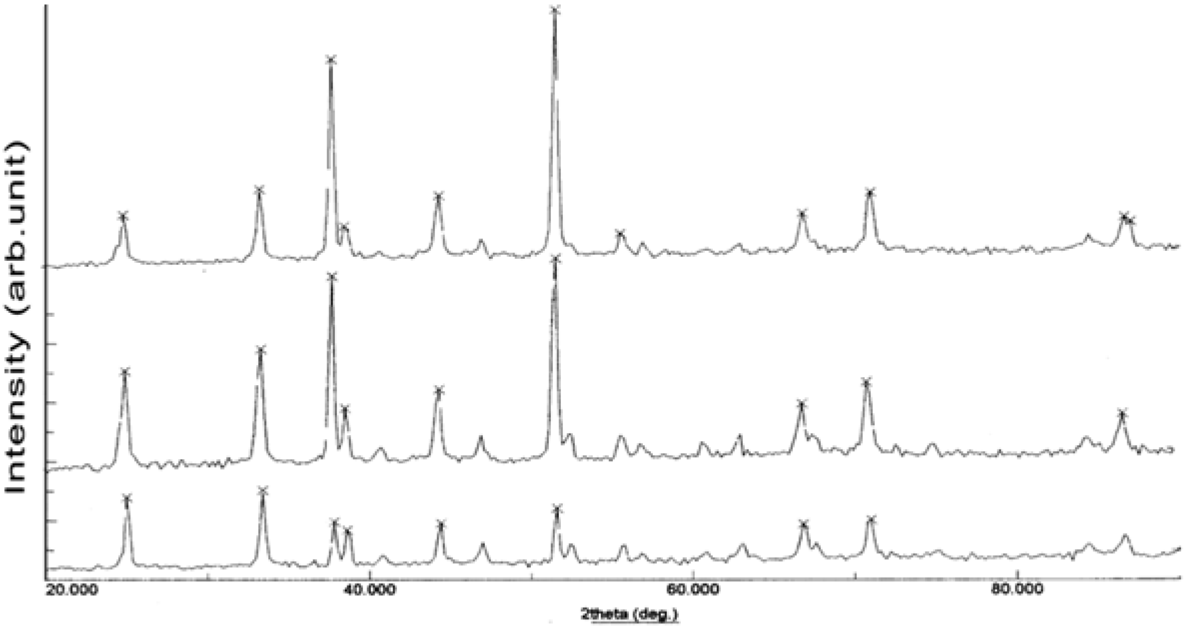


Figure 1 X-ray diffractogram of undoped PbI_2



Al-doped PbI2 (From top 0.1 M, 0.5 M &1M respectively)

Figure 2

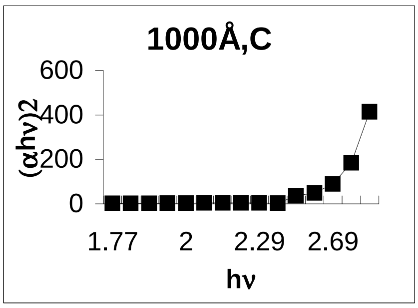


Fig.3: Transmission curve for undoped PbI_2

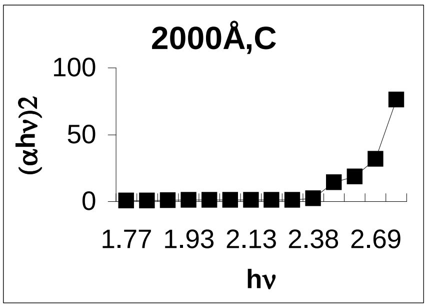


Fig.4: Transmission curve for undoped PbI_2

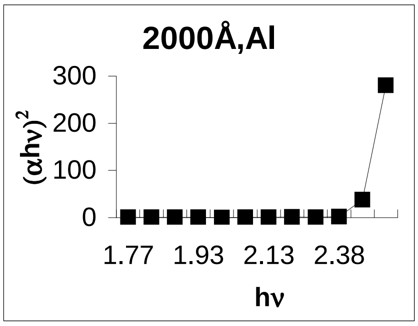


Fig.5: Transmission curve for Al-doped PbI_2

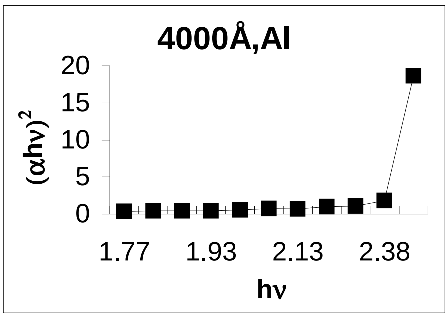


Fig.6: Transmission curve for Al-doped PbI_2

CONCLUSION

i) With proper doping in the Lead Iodide, 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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