Effect of Thickness on Physical Properties of Lead Iodide Crystals

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Abstract

Pure single crystals of lead iodide are grown by zone refining technique. After passing twenty five zones pure crystals are grown . Thin films of various thickness of these melt growth pure crystals are deposited by thermal evaporation technique .Resistivity, conductivity, and dielectric constants of films of various melt growth thickness are measured. From the investigation it is concluded that with increasing the film thickness conductivity increases and band gap, resistivity and dielectric constant decreases.

Introduction

Lead iodide is technically important class of material, in view of its band to band type of transition which make it very useful in several electronics and optoelectronic device applications. Lead Iodide is polytypic material. Different polytypes may serve as effective substitute for materials having specific physical properties. The investigation of electrical, optical and dielectric properties of lead iodide is thus of obvious significance.Some workers have reported that, the resistivity of melt growth lead iodide crystals is 4×10^{11} Ω cm) [1]and few reported that it varies from 4.1×10^{8} Ω cm- 4×10^{12} Ω cm [2]. Structure of lead iodide is hexagonal and atoms are located in layers of Pb and I perpendicular to c-axis. The sequence of layers is repeated in the units of I-Pb-I held together by van der Wall's forces. Lead iodide is wide bandgap (2.58ev) material][3,4].

Lead iodide converts X-ray energy directly in to electronic charges and due to electrostatic focusing of these charges, very good spatial resolution can be expected [5], so lead iodide can used as X-ray converter. Increasing interest has been focusing on the search for high-energy resolution room temperature X-ray detectors. The development of single detector spectrometers and, lately, of multidetector array systems has been driven by the specific needs of space exploration and synchrotron radiation applications[5].Lead iodide (PbI_2) crystals present an excellent response as X-ray detectors at room temperature[5].Band-gap energy and thermal properties of lead iodide were also determined by photo acoustic spectroscopy [6,7].

Many of physical properties of crystals depend on the presence of defects such as foreign atoms and native point defects .In order to study the effect of these defects on the physical properties, we require the starting material in which the concentration of such defects are as low as possible . The primary problem is therefore one of purification of starting material to remove foreign atoms. In the present case to solve this problem we used zone refining technique. The main advantage of zone- refining technique is that single crystal growth take place during the zone- refining process itself[8], and such melt grown crystals are polytypic [2].

In the present course of investigation, we have synthesized the Lead Iodide crystals by melt technique . In this paper the purpose of our studies is to check the effect of thickness of thin films on resistivity, conductivity and dielectric constant and band gap of purified lead iodide.

Experimental Details

In the present investigation the starting material was 99.9% pure supplied by M/s Aldrich. Further purification was achieved by using zone refining technique. This technique is fabricated in our laboratory. Twenty five zone passes were carried out to achieve maximum purity. The color of melt during zone refining was observed reddish black. The dark color of the melt could be due to excess of lead which is probably removed during the zone refining technique. Flow of argon was made to avoid the decomposition. Maximum purification is achieved by twenty five zone passes .The pure crystals grown by this technique are transparent and yellowish in color. Conductivity and resistivity are measured by using Kithely electrometer(Model-6517) and dielectric constant is measured by Kithely LCZ meter (Model-3330). Vacuum thermal evaporation is used for preparation of thin films. It is carried out in vacuum of 1 micron and source material is heated by an electric filament. In this technique vaporization of solid material(by heating to sufficiently high temperature)and condensing it on cooler substrate takes place to deposit the thin films. Purified lead iodide is placed in tungsten boat for the deposition of thin films. Thin films of various thickness were deposited on the glass substrate by using vacuum coating unit (MODEL EYU-3000S,VEQCO) keeping the substrate at room temperature in vacuum of 10-5 torr .Thin films were kept inside the vacuum chamber for 15 hours .The quartz crystal thickness monitor was used for monitoring the film thickness during evaporation. The deposition rate was slow (2-3 nm/s), as higher deposition rate led to non-uniform growth and low sticking. The films of thickness below 30 nm were non uniform , discontinuous and above 500nm peel of the substrate. The optical absorption measurement were carried out in UV/VIS region by using JASCO-570 spectrometer.

Result and Discussion

For the study of various properties only small section of single crystal were required. This could be obtained from zone purified material. A small single crystal section removed from the twenty five pass material was used as seed . The seed was placed at the initial end of purified material . A small portion of material was melted and the zone was moved towards the seed until a part of seed melted in to molten pool. The zone was then quickly reversed and the crystal allowed to grow. In this way single crystal of purified lead iodide material grow. The purified crystal was golden yellow in color. In a crystalline or polycrystalline material both direct or indirect optical transitions are possible depending on the band structure of material[9]. Assuming parabolic bands, the relation between absorption coefficient (α) and band gap E_g for a direct transition is given by[10].

$$\alpha h\nu = \text{constant}(h\nu - E_g)^n$$

Where α is absorption coefficient of material, hν is photon energy and E_g is band gap of material. For a direct transition n=1/2 or3/2 depending upon whether the transition is allowed or forbidden in quantum mechanical sense.The usual method of determining the band gap is to plot a graph between $(\alpha h\nu)^{1/2}$ and hν. In the present case ,n=1/2 gives best graph in the band edge region.

In general , thickness dependence of band gap arises due to one or more combined effect of the following causes: large density of dislocations, quantum size effect and the change in barrier height due to change in grain size in polycrystalline films.

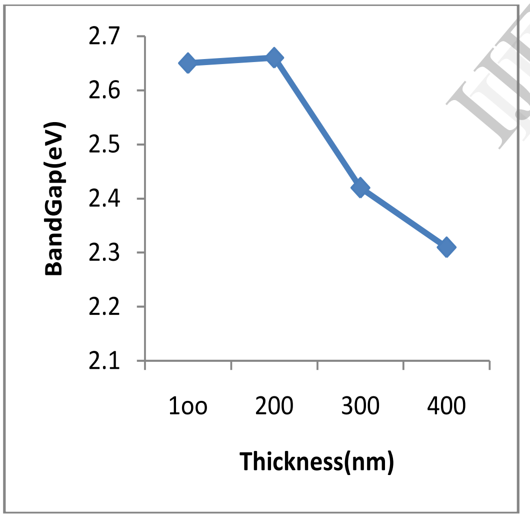

Fig1:Variation of band gap with thickness of film

However, first one not looks the reasonable cause in the present case with small contributions from dislocations density as well. In the present case the thickness of films is quite large , so the quantum size effect can completely ruled out. The band gap decrease with increase

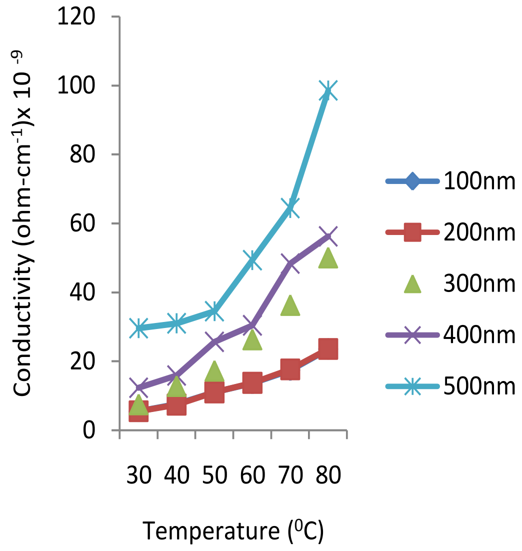

Fig. 2:Variation of conductivity with thickness of film

in the grain size because barrier height decrease[11]. It is clear from the Fig -1,the band gap variation with thickness is nominal for thickness less than 200 nm this could be due to better alignment of grains as film thickness become larger, the misalignment among the grains starts leading to grain boundary structure[12]. Lead iodide is wide band gap material which converts X-ray energy directly in to electronic charges. Due to electrostatic focusing of these charges , very good spatial resolution can be expected [6], so lead iodide can used as X-ray converter.

Since the band gap decreases with increasing the film thickness, so conductivity also increases and resistivity decreases with increasing the film thickness as shown in Fig.2-3.

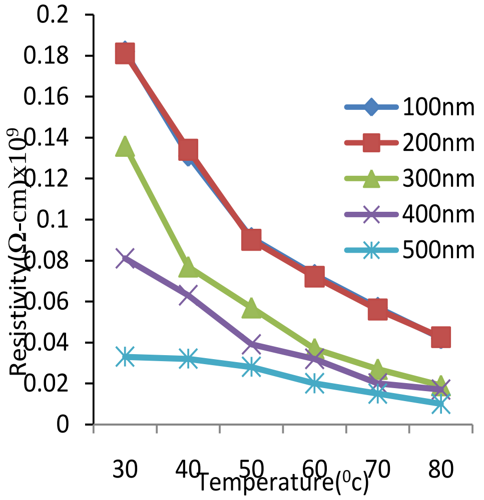

Fig. 3:Variation of resistivity with thickness of film

Resistivity of led iodide crystals was estimated to be of order of 10^9 ohm-cm. This result is very encouraging because due to such high resistivity ,the noise due to dark current is minimal[5]. The dielectric response with frequency for lead iodide is shown in Fig.4.

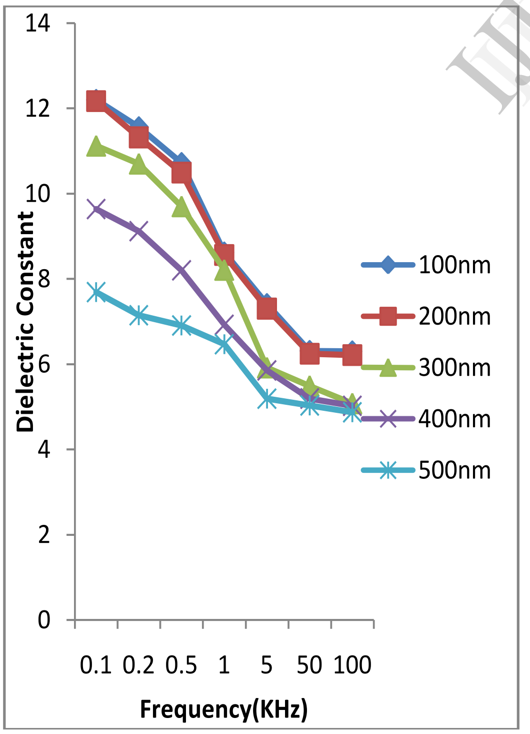

Fig.4:Variation of dielectric constant with thickness of film

Lead iodide is layered structured crystal and dipoles are free for orientations, so orientations of dipoles are changed with frequency. After increasing the film thickness, decrease in dielectric constant indicates that there is no considerable polarization effect, because the misalignment among the grains starts .

Conclusion

From the above discussion we conclude that , lead iodide material is purified using zone refining technique and pure crystals of lead iodide are grown after twenty five zone passes. From this purified material thin films of various thickness are deposited. In the present investigation it is concluded that conductivity increases, while resistivity band gap and dielectric constant of lead iodide decreases with increasing the film thickness .

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