EFFECT OF PURITY OF CADMIUM IODIDE CRYSTALS ON PHYSICAL PROPERTIES

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ABSTRACT

Cadmium iodide crystals are polytypic in nature. Pure single crystals of cadmium iodide are grown by zone refining technique. After passing twenty five zones pure and single crystals of CdI_2 are grown. Resistivity, conductivity , dielectric constant and band gap of cadmium iodide are measured after 8^{th},15^{th} and 25^{th} Zone passes. From this study it is concluded that resistivity, dielectric constant and band gap decreases after each zone passes while conductivity increases ,because presence of stacking faults in impure crystal.

Key Words: CdI_2; Resistivity; Conductivity; Dielectric constant

1. INTRODUCTION

CdI_2 is layer structured compound with hexagonal sheet of Cd atoms sandwiched between two similar sheet of I atoms .Its crystals are known to be rich in poytypism .Cadmium iodide being one of the most thoroughly investigated compound of halide family, it is not surprising that a wealth of information is available on CdI_2. Virtually all the components of commonly known techniques have been applied to obtain this material in single crystal form. CdI_2 is known to bean ionic compound and the I ions are much larger than Cd ions. 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. Single crystals of lead iodide have been grown by aqueous solution, gel, melt, sublimation and chemical vapor transport. In the present work crystal is grown by melt technique (zone refining technique). The main advantage of zone- refining technique is that single crystal growth take place during the zone- refining process itself [1]. The reported result revealed that only pure 4H polytype was obtained [2]. X-ray studies [3], electrical and optical characterization [4], recombination process [5] of cadmium iodide have been reported.

2. EXPERIMENTAL DETAILS

In the present investigation the starting material was 99.9% pure supplied by M/s CDH. Further purification was achieved by using zone refining technique. This technique is fabricated in our laboratory. The main chamber is consisted of a pyrex glass tube with a diameter of 3 cm and length 60 cm. one end of the tube is connected to an argon cylinder and the other end is connected to a coaxial brass tube. To escape argon cloud the open end of this tube is dipped in to water. Flow of argon is made to avoid the decomposition. Twenty five zone passes were carried out to achieve maximum purity. The color of melt during zone refining is observed grey. Zoning was made more rapid by using a speed of 5 cm/h. Purification involves repeated passage of molten zone. The pure crystals grown by this technique are white in color. For measuring resistivity, conductivity and dielectric constant only small section of single crystal is required. Conductivity and resistivity are measured by using Kithely electrometer (Model-6517) and dielectric constant is measured by Kithely LCZ meter (Model-3330).Optical absorption measurement is carried out in UV/VIS region by using JASCOV-570 UV/VIS/NIR spectrometer.

3. 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. After just two zone passes, some clearly visible specks of impurities were found to be accumulated at far end of boat. During purification the impurities which are more soluble in the melt, move along the direction of movement of molten zone and the impurities which are less soluble in the melt, move in a direction opposite to that of molten zone. More passes are therefore needed to move the latter impurities. A small single crystal section removed from the twenty five zone passes 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 cadmium iodide material grow. When atoms come together to form a solid, their valence electrons interact due to coulomb forces, and they also feel the electric field produced by their own nucleus and that of the other atoms property (which include the energy). In solids, there is an energy gap between the valence and conduction band, so energy is needed to promote an electron to the conduction band. This energy may come from heat, or from energetic radiation, like light of sufficiently small wavelength. In a crystalline or polycrystalline material both direct or indirect optical transitions are possible depending on the band structure of material[6].

Assuming parabolic bands, the relation between absorption coefficient (α) and band gap E_g for a direct transition is given by[7].

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

Where α is absorption coefficient of material, $h\nu$ 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 $h\nu$. In the present case ,n=1/2 gives best graph in the band edge region.

The band gap is decreased with increasing the zone passes or with increasing the purity of crystals . The impure crystal contains stacking faults and has short range order of periodicity. So as compared to impure crystal, in a pure crystal most of the incoming radiation would be absorbed by the electrons and be excited from the valence band into the conduction band. Such materials are very effective in narrowing the photon distribution. Only photons with energy greater than band gap of the materials will be absorbed. With increasing the number of zone passes band gap and resistivity decreases i.e. band gap and resistivity measured after 8^{th} zone passes is greater than measured after 15^{th} zone passes and 15^{th} zone passes is greater than measured after 20^{th} zone passes (Fig .1and2) The resistivity of cadmium iodide is of order of 10^{10} ohm-cm. This result is very encouraging because due to such high resistivity, the noise due to dark current is minimal [8].

Since the electrical conductivity is the inverse of the resistivity ($\sigma = 1/\rho$) due to decrease in band gap, conductivity of pure crystal is higher than less pure or impure crystal (Fig.3).

The dielectric response for different zone passes at different frequency is shown in Fig .4. Cadmium iodide is layered structured crystal and dipoles are free for orientations, so orientations of dipoles are changed with frequency. From dielectric response curve it is clear that dielectric constants reduced rapidly with increasing the frequency because orientations of dipoles are diverted with frequency. There is no considerable polarization effect after purification, so there is a decrease in dielectric constant.

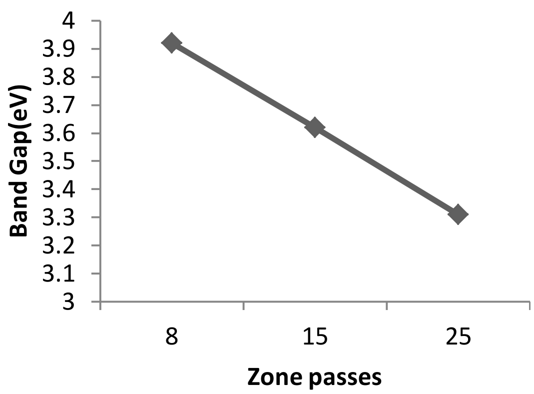

Fig.1: Variation of band gap v/s Zone passes

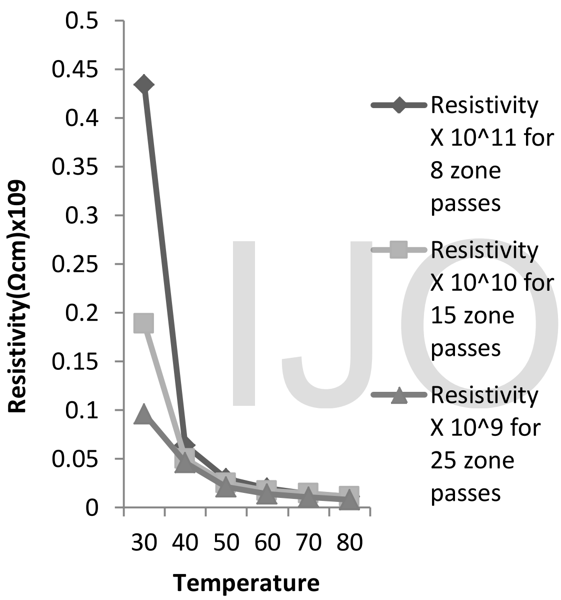

Fig.2: Variation of resistivity with zone passes

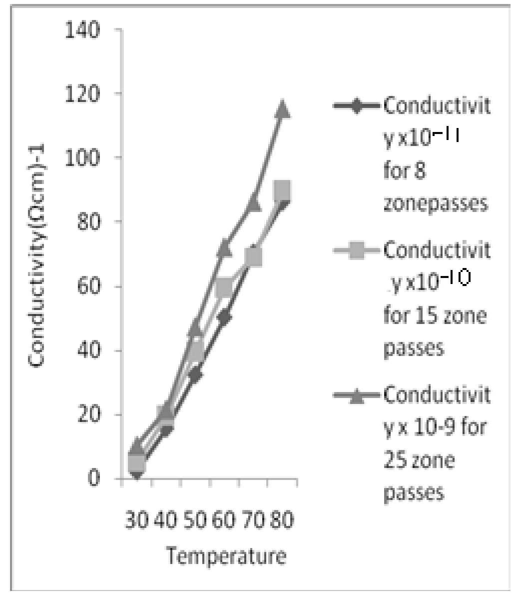

Fig. 3: Temperature v/s Conductivity with Zone passes for CdI_2 crystal

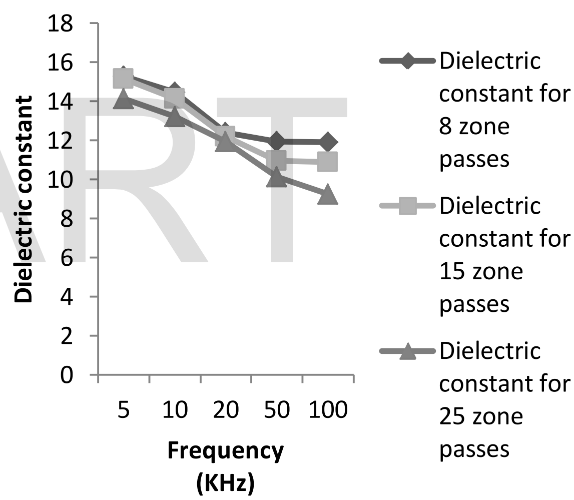

Fig.4: Variation of conductivity with zone passes

4. CONCLUSION

Cadmium iodide material is purified using zone refining technique and pure crystals are grown after twenty five zone passes. The band gap, resistivity and dielectric response graphs show that these quantities have smaller value for pure crystal as compared to lesser pure crystals, while value of conductivity is higher for pure crystal.

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