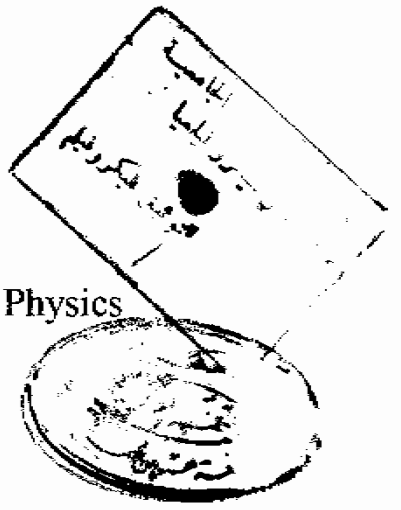
THE STRUCTURAL AND TRANSPORT PROPERTIES OF CADMIUM ARSENIDE THIN FILMS (Cd_3As_2)



THESIS

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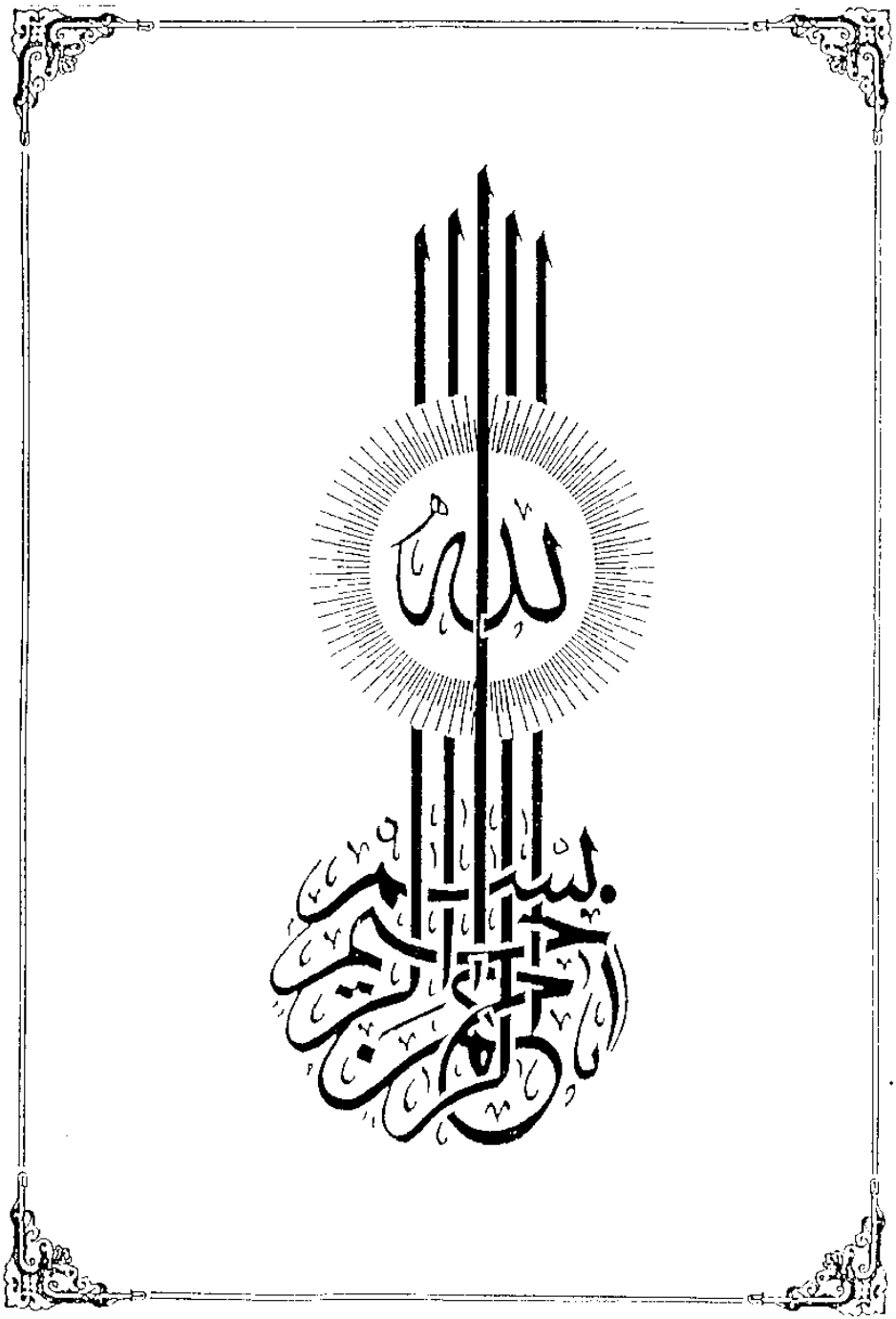

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ABSTRACT

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It was found throughout this work that all Cd_3As_2 thin films, whatever the film thickness in the thickness range of 50.5 nm - 200 nm and whatever the deposition rate up to 5 nm s^{-1}, have polycrystalline nature of tetragonal structure. The obtained lattice constants are:

a = 12. 54 ± 0.13 Å and c = 25.51 ± 0.93 Å belonging to the α - phase. It was also found that the size of the individual grains increases with increasing the film thickness up to 90 nm over which the size of the individual grains becomes approximately constant. Increasing the deposition rate decreases the degree of crystallinity. At a deposition rate 5 nm s^{-1} the Cd_3As_2 films have amorphous nature.

Concerning the optical properties of Cd_3As_2 polycrystalline thin films, the optical constants i.e., the refractive index n and the absorption index k were determined in the spectral range of 0.5 μm - 10 μm. It was found that the discrepancy in either the refractive index or the absorption index lies within the limits of experimental error, so both n and k are practically independent on the film thickness in the thickness range of 48.9 - 138.4 nm. It was obvious that the refractive index n of Cd_3As_2 polycrystalline thin films shows an anomalous dispersion in the spectral range below 1000 nm. The lattice dielectric constant ε_L for these films is found to be 17.6. Graphical representation between log ($\alpha h\nu$) and log ($1/\lambda$) yields three distinct linear regions. The first region is the photon energy range up to 0.3 eV. The second region is the photon energy range of

0.3 - 0.95 eV. The third region is the photon energy range of 0.95 - 2.1 eV. Graphical representation of $\alpha h\nu \sim (h\nu - E_g)^r$ in each of these regions indicates the type of the allowed optical transitions that can exist. It was found in the first region that the only allowed type of optical transitions are indirect allowed optical transitions with energy gap $E_g^{ind} = 0.05$ eV. In the second region, the only allowed type of optical transitions are direct allowed optical transitions with energy gap $E_g^{d} = 0.72$ eV. In the third region, the only allowed type of optical transition are direct allowed optical transitions with energy gap $E_g^{d} = 1.56$ eV. The last two values were confirmed throughout the graphical representation of either the volume or surface energy loss function. This graphical representation yields two peaks, one at 0.73 eV and the other at 1.53 eV. The first peak can be attributed to tetragonal splitting of the P-like valence band at Γ point. The second peak can be attributed to allowed direct transitions $\Lambda_3 \rightarrow \Lambda_1$ according to Lin-Chung model. According to this model the indirect optical transitions are expected between $\Gamma_1 \rightarrow \Gamma_{15}$.

With respect to transport properties of Cd_3As_2 polycrystalline thin films, it was found that both the dark electrical resistivity (ρ), Hall coefficient and Seebeck coefficient measurements indicate that Cd_3As_2 films in polycrystalline form behave as a degenerate semiconductor. The last two parameters indicate that it is n-type semiconductor. The data representing the resistivity ρ versus the film thickness t was examined on the basis of both F-S and M-S theories. It was found that there is a considerable agreement between the present experiment results and M-S theory.

The dark electrical resistivity of Cd_3As_2 polycrystalline films was found to be independent upon the film temperature up to about 400 K, which is an obvious feature of degeneracy.

The measured values of the Hall coefficient as a function of the film thickness or as a function of the deposition rate were used to calculate the electron concentration and the electron mobility. The electron concentration was found to have the order of 10^{24} m^{-3}.

The Seebeck coefficient S measurements lead to confirm the conduction mechanisms as they show, throughout the graphical representation of S versus (1000/T), that there are two different mechanisms which are the ionized scattering mechanism in lower temperature range and lattice scattering mechanism in relatively higher temperature range.

Seebeck coefficient measurements as a function of (1000/T) can also be used in conjunction with the optical energy gaps to determine the ratio between the mobility of electrons and the mobility of holes. It was found that $\mu_n > \mu_p$. This is required for the n-type semiconductors.

The electron concentration calculated from Hall coefficient measurements was used in conjunction with the reduced Fermi energy calculated from the Seebeck coefficient measurements to calculate the electron effective mass of Cd_3As_2 polycrystalline thin films. It was found that $m^* = 0.053\ m_o$ where m_o is the rest mass of the electron.

To obtain the above mentioned results the coming experimental techniques were followed .

To investigate the crystalline structure of the thin Cd_3As_2 films ,both X-ray and electron diffraction techniques were utilized.

The optical constants were determined on the basis of two physical quantities which are the reflectance and transmittance of any Cd_3As_2 thin film measured at normal incidence at room temperature using two spectrophotometers (Cary 2390 ,Varian Co.) in the wavelength range of 0.5-2.3 μm and (PYE Unicam Sp. 3-300) in the wavelength range of 2.5-10 μm.

The dark electrical resistivity of Cd_3As_2 thin films was measured using the two points probe method.

A D.C. technique was utilized in measuring the Hall voltage drop across two specified terminals. Tinsley potentiometer UJ33E with accuracy ± 0.1 μV was used as a null detector.

The differential method was used for measuring the thermoelectric power of Cd_3As_2 thin films. The thermoelectric power of any sample was measured using highly internal impedence electrometer (Keithley 616 A) .

The film thickness was measured using multiple- beam Fizeau fringes.

INTRODUCTION

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The II-V compound cadmium arsenide (Cd_3As_2) has been of great interest since it was found to be a semiconductor of small energy gap, high carrier mobility and low electron effective mass. This compound is characterized by its high transmittance over a broad range of the IR spectrum. Its electric and thermoelectric properties make it suitable for use in thin film Hall generator, photo detectors.

In spite of a continuously increasing number of publications concerning the optical and electrical transport properties of Cd_3As_2 either in bulk form or in thin film form, there continue to be a lack of agreement on the energy band structure of Cd_3As_2 especially on the nature of the fundamental absorption edge. So, accurate experimental investigations of the electrical and especially the optical properties are needed to establish the true energy band structure of this compound and for quantitative comparison. Accordingly, the aim of the present work is devoted to investigate:

1) The micro structure of Cd_3As_2 thin films prepared either by flash evaporation or by thermal evaporation. This investigation includes the structural dependence of the following parameters:

   (i) The film thickness.

   (ii) The deposition rate.

   and

(iii) The annealing temperature.

2) The optical properties of Cd_3As_2 in thin film form. This investigation includes:

(i) The determination of the optical constants in a considerable range of spectrum.

(ii) The determination of the allowed type of the optical transitions that may occur in Cd_3As_2 thin films.

(iii) The determination of the energy gap of any existing allowed optical transitions, whether the observed type (direct or indirect) of the allowed optical transition is really existing or not.

3) The electrical transport properties of Cd_3As_2 thin films. This investigation includes:

(i) Electrical resistivity measurements in dark.

(ii) Hall coefficient measurements.

and

(iii) Seebeck coefficient measurements.

4) Interpretation of the obtained results.

CHAPTER I

THEORETICAL BACKGROUND AND LITERATURE REVIEW

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THEORETICAL BACKGROUND AND LITERATURE REVIEW

The present chapter is devoted to the theoretical background and the literature review concerning the followings:

* Structural properties of Cd_3As_2

* The energy band structure of Cd_3As_2

* Transport properties of Cd_3As_2

* Optical properties of Cd_3As_2

These items are given in detail in the following

I.1) Structural Properties of Cd_3As_2

I.1.1) Structural Properties of Cd_3As_2 in Bulk Form:

The crystal structure of Cd_3As_2 was determined by Von Stackelberg and Paulus[1] as tetragonal with a=8.95 Å , c=12.65 Å, and c/a = 1.418 belonging to the space group $P4_2/nmc$ with As-ions approximately in a cubic close-packed array. Cd ions were tetrahedrally coordinated and each As ion was surrounded by Cd ions at six of the eight corners of a distorted cube, the two vacant sites being at diagonally opposite corners of a cube face.

Stoichiometric quantities of cadmium and arsenic were heated in a sealed evacuated silica tube at 950 K for 18 hours. The sample was then heated at 1125 K for two hours prior to air quenching. The resulting polycrystalline mass was found to contain single crystals sufficiently large for study by the Weissenberg technique. Weissenberg photographs of a suitable single crystal carried out by Steigmann et al[2] by single crystal analysis indicated a body-centered tetragonal cell approximately four times the size of the cell found by Von Stackelberg and Paulus. An accurate determination of the lattice parameters, obtained from powder data taken with CuKα- radiation and a crystal-focusing camera of effective diameter 22.9 cm, gave a=12.67±0.01 Å and c=25.48±0.02 Å. Steigmann and Goodyear[2] reported that the disagreement between their structural data and those