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Structural And Transport Properties of Some Ternary Compounds

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ABSTRACT: Crystals of $AgInTe_2$ (AIT) were grown by Bridgman technique method. The crystals were identified structurally by using X-ray diffraction technique. Measurements of electrical conductivity and Hall effect were performed in the wide temperature range (165-600 K). Thermoelectric power measurements were carried out in the temperature interval (182-408K). From these measurements, many various physical parameters were determined. The energy gap has been estimated to be 1 eV and the type of conductivity was found to be n-type. Crystallite size (D) of the obtained $AgInTe_2$ crystals was calculated to be 166.6 nm. A detailed discussions were done on the basis of the crystal structure of the crystals. The lattice parameter a, b and c for the prepared crystals were calculated.

Keywords: $AgInTe_2$, crystal growth, X-ray diffraction, electrical properties.

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I. INTRODUCTION

Among the I–III–VI family of semiconducting materials, $AgInTe_2$ (AIT) with a direct energy band gap of 1.04 eV, has potential applications in photovoltaic energy conversion because of their diverse optical, electrical, and structural properties [1]. The electrical properties of nearly homogeneous samples of $AgInTe_2$ have been examined between 100 and 300 K [2]. The structural, electrical and optical properties of AgInTe2 films have been reported [3-7]. A theoretical study of the thermal and structural properties of chalcopyrite $AgInTe_2$ has been presented [8] and photoluminescence characteristics of polycrystalline chalcopyrite $AgInTe_2$ was investigated [9]. However the pre-mentioned work was done in a limited temperature range, $AgInTe_2$ (AIT) one of the less studied ternary chalcopyrite compound and literature still lacks work that focuses explicitly on transport properties of $AgInTe_2$. Accordingly, In the present work, the transport properties of homogeneous samples of n-type $AgInTe_2$ have been widely studied. From this analysis much information about the relevant physical parameters of $AgInTe_2$ in a wide temperature range have been estimated.

II. EXPERIMENTAL PROCEDURES

2.1. Growth technique

By using Bridgman modified method, the crystals of $AgInTe_2$ were grown. According to this technique, the samples have been prepared by the direct melting of the starting materials (Ag , In, and Te) in quartz ampoule which was sealed under vacuum of $\approx 10^{-4}$ Torr. The silica ampoule and its charge were mounted in the first zone of a three-zone tube furnace. The temperature in the first zone was higher than the melting point and then the temperature was kept about 24 h for complete melting and mixing the starting materials. The temperature of the middle zone of the furnace was 929 K corresponding to the crystallization temperature of $AgInTe_2$ as reported in the phase diagram [10]. When the ampoule and the melt entered the third zone gradually, solidification has been occurred since the temperature was adjusted to be less than the melting point.

2.2 Electrical conductivity and Hall effect measurements

Samples of rectangular form of 12x4.24x1.8 mm^3 dimensions were used for performing the electrical conductivity and Hall coefficient measurements according to calculated correction factors [11]. A pyrex cryostat, which was designed in our laboratories [12] was used for adjusting the low temperature (with the aid of liquid nitrogen) and high temperature was achieved via an electric heater. The cryostat, which contains the crystal, was evacuated (10^{-4} Torr) for avoiding vapour water condensation or crystal oxidation.

2.3 Thermoelectric Power Measurements

Measurement of the thermoelectric power has been done by using a pressure contact sample holder. Also an evacuated calorimeter (10^{-4}Torr) was used to protect the sample from oxidation and water vapor condensation at high and low temperatures, respectively.

III. RESULTS AND DISCUSSION

3.1 Structural analysis

Fig. 1 depicts the X-ray diffractogram for the prepared $AgInTe_2$ crystals. The spectrum confirm the crystalline nature of the prepared crystals. XRD measurements showed agreement with ASTM cards. The powder XRD analysis confirmed the synthesis of tetragonal $AgInTe_2$.The lattice parameters a and c of grown crystals $AgInTe_2$ has been calculated by plotting the lattice parameters, a_{hkl} and c_{hkl} (calculated from the Bragg's Law of the main peaks) against an extrapolation function $F(\theta) = [\frac{1}{2}(\cos 2\theta / \sin\theta + \cos 2\theta/\theta)]$ which holds quite accurately down to low values of θ. Fig. 2 shows the relation between the lattice a and F(θ). The estimated values of lattice parameter of $AgInTe_2$ tetragonal phases, are a=6.599 Å and c = 12.37Å, which are in good agreement with the values found in the literature [13].

Crystallite size (D) of the obtained AgInTe2 crystals was calculated to be 166 .6 nm from the Debye–Scherrer's formula [14]

$$D = \frac{0.94\,\lambda}{\beta \cos\theta} \qquad (1)$$

where λ is 1.54056 Å for CuKα. β is the full width at half maximum (FWHM) of the line, and θ is the diffraction angle.

3.2. Electrical Conductivity and Hall Measurements

The variation of σ against $10^3/T$ was illustrated in Fig. (3). The curve is divided into three parts, in the first part σ increases slowly, the impurity ionization energy ΔE_d was 0.32 eV. In the second region the fall in the electrical conductivity was observed. Then the intrinsic conduction appears (as seen from the figure) where σ increases sharply. The following equation is used to estimate the value of the energy gap,

$$\sigma = \sigma_0 \exp(-\Delta E_g/2\, k_B T) \qquad (2)$$

The energy gap was found to be 1 eV. The electrical conductivity at room temperature amounts to be as 0.78 ohm $^{-1}$cm^{-1}.

Fig. (4) depicts the relation between $R_H T^{3/2}$ and $10^3/T$. The two regions have been distinguished according to the relation:

$$R_H T^{3/2} \propto \exp(-\Delta E_g/2\, k_B T) \qquad (3)$$

From the figure and the above formula the values of the energy gap have been estimated. These values are found in a good agreement with these obtained from the electrical conductivity measurements. At room temperature R_H has a value of 1296 cm^3 /C. Measurements of the Hall coefficient and the electrical conductivity made it possible to detect the effect of temperature on the Hall mobility. The temperature dependence on the Hall mobility μ_H shown in Fig.5. At low temperatures (T< 303K), μ_H increases with temperature following the relation $\mu \alpha T^{12}$.Such behavior is the characteristic of a scattering mechanism of the charge carriers with ionized impurities. While at the high temperature (T>303K), mobility decreases with increasing temperature according to $\mu \alpha T^{-5.6}$,This may be due to the interaction between charge carriers and phonons which is dominant. At room temperature, Hall mobility equals 1011 cm^2/Vs. As a complementary part to the Hall work; the mode of variation of the charge carrier concentration against temperature was checked. Fig (6) shows such behaviour. From this relation the energy gap width was found to be 0.98eV. The value of the charge carrier concentration at room temperature is 4.8×10^{15} cm^{-3} .

3.3 Thermoelectric Power Measurement

The thermoelectric power (TEP) measurements of $AgInTe_2$ were carried out as a complementary part to the electrical conductivity and Hall effect. The relation between thermoelectric power (α) and the temperature is depicted in Fig.7. From this figure, we can see that α increases with temperature up to its maximum value (276 μV/K) at a temperature 303 K. Above 303 K, α decreases. The growth of α with T is due to the thermal activation of the charge carriers. At T = 303K (the maximum value of α) the intrinsic conduction appears. The decrease of α above 303 K is due to the compensation process which takes place in this range of temperature. TEP of the $AgInTe_2$ sample has a negative sign over the entire considered temperature range. The value of

thermoelectric power at room temperature is 276 μV/K. The following equation in the intrinsic region can be applied [15]:

$$\alpha = \frac{K}{e}\left[\frac{b-1}{b+1}\left(\frac{\Delta E_g}{2KT}+2\right)+\frac{1}{2}Ln\left(\frac{m_n^*}{m_p^*}\right)^{3/2}\right] \qquad (4)$$

Where $b = \mu_n / \mu_p$, ΔE_g is the energy gap, K is the Boltzman constant. m_n^* the electron effective mass and m_p^* the hole effective mass. Taking into consideration the value of ΔE_g=1 eV (as obtained from the electrical conductivity measurements in the same range of T, the ratio of the electron and hole mobility was calculated from the slope of the line in the high temperature range of Fig. 7 and was found to be 1.14. By considering the value of μ_n = 1011 cm^2/Vs which was obtained from the Hall measurements data, the value of μ_p was estimated to be 887 cm^2/Vs. Meanwhile, the ratio m_n^*/m_p^* was also calculated from the intercept of the curve with α-axis and was found to be 0.33.

In the extrinsic region the next equation was employed [16]:

$$\alpha = \frac{K}{e}\left[2 - Ln\frac{nh^3}{2(2\pi m_n^* KT)^{3/2}}\right] \qquad (5)$$

The relation between α and lnT according to this equation was drawn. Then from the intercept of the line (in the impurity region) with the α-axis, we got m_n^* =7.7x10^{-33} kg. Taking into account the ratio previously obtained from Fig. 7, we evaluated m_p^* as 2.34x10^{-32} kg. The value of the relaxation time for electrons was 1.27x10^{-10} s. It was calculated according to the equation $(\tau_n = \mu_n m_n^*/e)$, while for holes it is 4.8x10^{-11} s. Furthermore, the diffusion constants for electrons and holes were calculated and found to be D_n = 26.15 cm^2/s and D_p = 22.9 cm^2/s, respectively $(D_n = (k_B T \mu_n / e)$. The diffusion length L_n and L_p were also calculated and found to be 3.54x10^{-5} cm and 5.4x10^{-5} cm for electrons and holes, respectively $(L_n = (D_n \tau_n)^{1/2})$.

Fig. 8 shows the dependence of thermoelectric power on the charge carriers concentration n which follows the equation [17]

$$\alpha = \frac{\kappa}{e}\left[A + Ln\frac{2(2\pi m_n^* KT)^{3/2}}{(2\pi h)^3}\right] - \frac{\kappa}{e}\ln n \qquad (6)$$

Where A is a constant depending on the scattering mechanisms.

The similar behavior in Fig. 7 and Fig. 8 suggests that the variation of α may be to the variation of carrier concentration with temperature. Figure (9) shows the Seebeck coefficient (α) versus logarithm of electrical conductivity (ln σ), according to the relation [18]. Also The behavior of the curve for the relation between electrical conductivity and α is similar to that of α versus n.

IV. CONCLUSION

$AgInTe_2$ crystals were grown by Bridgman technique. The results of investigations were carried out to determine the structural, electrical and thermoelectric power properties of the obtained $AgInTe_2$ crystals. From these measurements, many physical parameters were estimated.Crystallite size (D) of the $AgInTe_2$ crystals was calculated to be 166.6nm. The estimated values of lattice parameters of $AgInTe_2$ are a=6.599 Å and c = 12.37Å. The energy gap was found to be 1eV. Conductivity type was found to be n-type.

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Fig (1) X-RAY diffraction pattern for $AgInTe_2$.

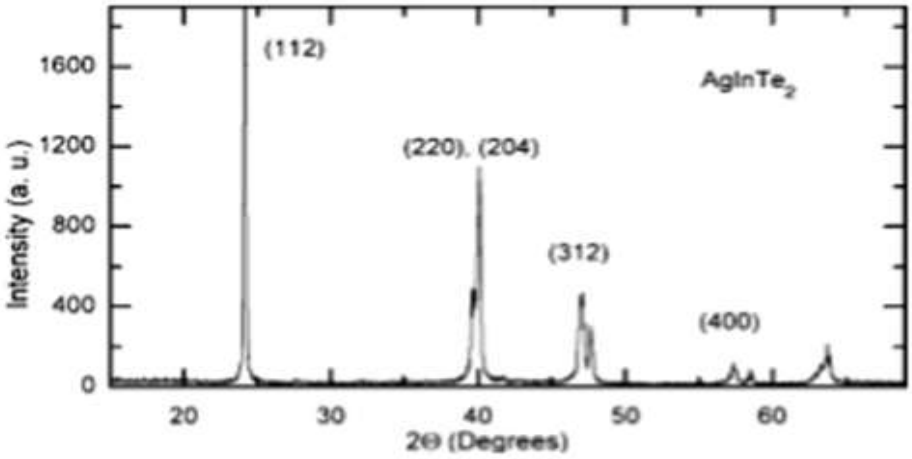


Fig (2). The relation between the lattice parameter (a) and F(θ) for AgInTe2.

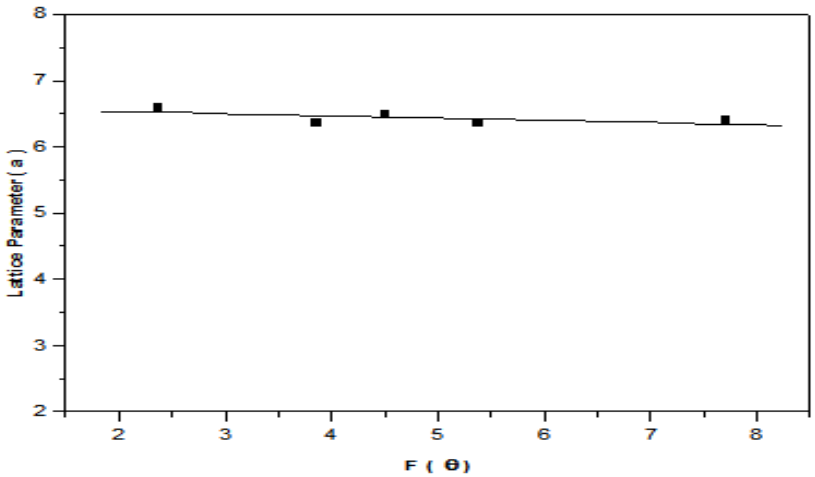


Fig. (3) Temperature dependence of σ for $AgInTe_2$.

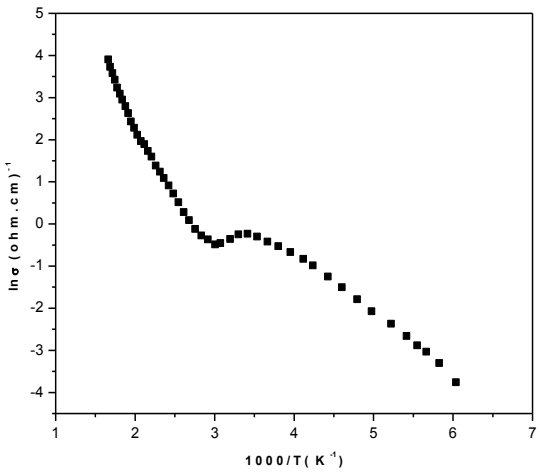


Fig. (4) Temperature dependence of Hall coefficient $R_H T^{3/2}$ for $AgInTe_2$.

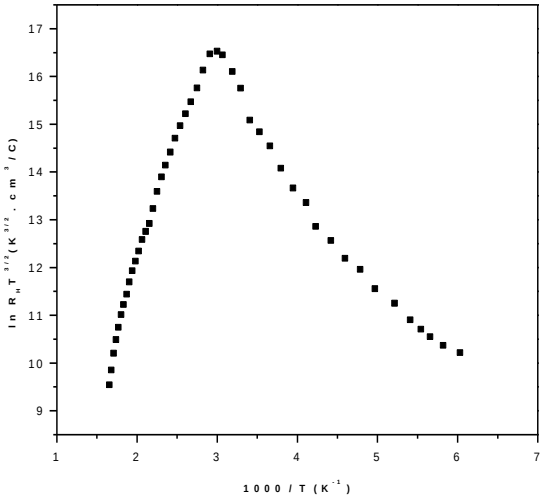


Fig. (5) Behavior of μ as a function of temperature for $AgInTe_2$.

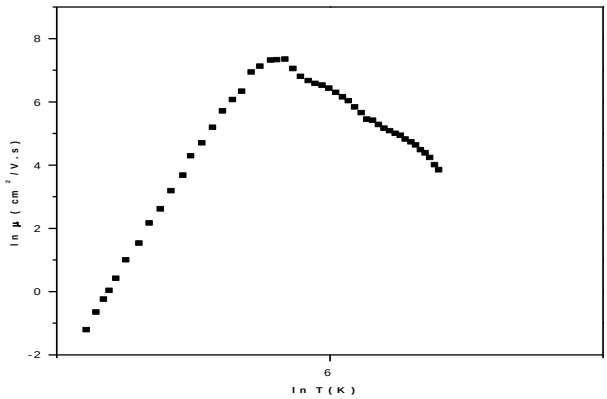


Fig. (6) Variatation of carrier concentration with temperature for $AgInTe_2$.

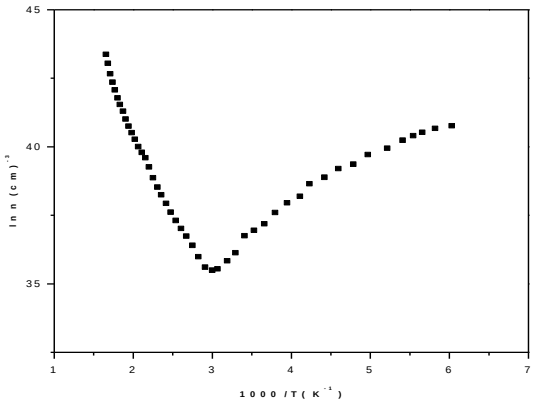


Fig. (7) Relation between thermoelectric power(α) and 1000/T for $AgInTe_2$.

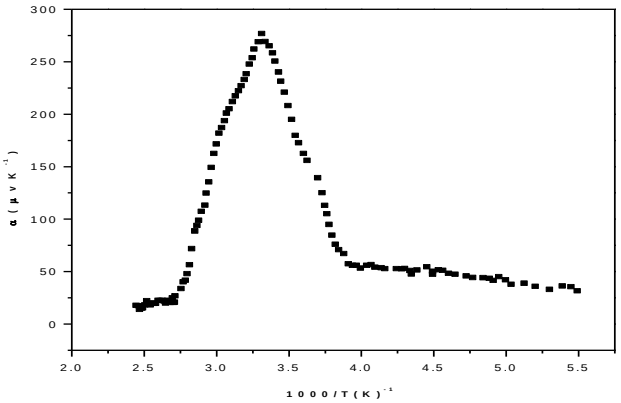


Fig. (8) Thermoelectric power dependence of charge carrier concentration for $AgInTe_2$.

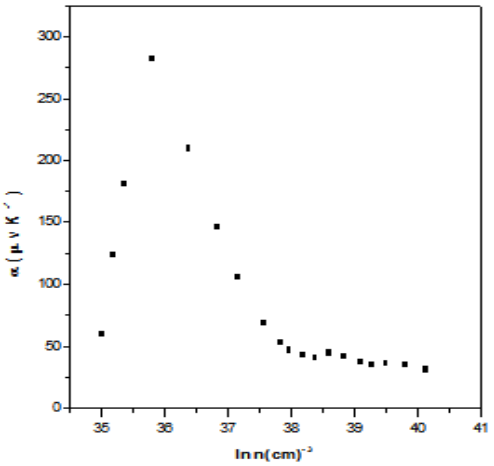
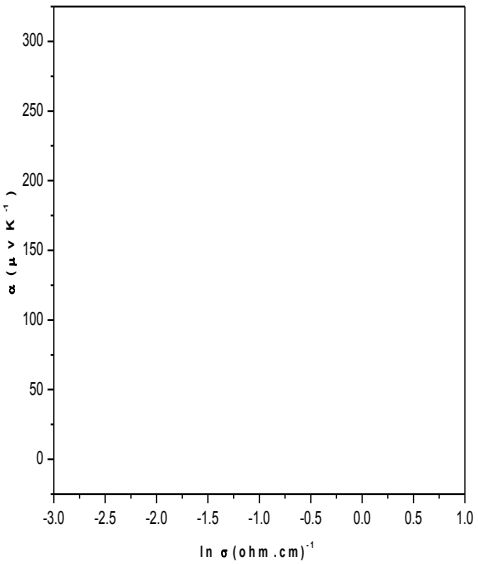


Fig. (9) Variation of (α) vs. (σ) for $AgInTe_2$.



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