Investigation of the Electrical Transport Properties of $TlBiTe_2$ Single Crystals

F.S.Bahabri[1], A.T.Nagat[1], R. H. Al-Orainy[1], F. S. Shokr[1], S.A.Al-Gohtany[1] and M. H. Al-Husuny[2]

[1.] Physics Department, Science of Faculty for Girls, King Abdul Aziz University- KSA
[2.] Physics Department, Science of Faculty for Girls, Tuyba University - KSA
f_s_bahabri@hotmail.com

Abstract: The preparation and electrical properties of a Thallium Bismuth ditelluride single crystals are reported in the present work. Measurements of the electrical conductivity and Hall coefficient were performed over a temperature range from 178-568 K. The study was carried out under vacuum. The crystals obtained had p-type conductivity with a hole concentration of 1.4×10^{10} cm^{-3} at room temperature. The conductivity and Hall mobility at 300K were 5.06×10^{-6} $\Omega^{-1}cm^{-1}$ and 2257.53 $cm^2V^{-1}s^{-1}$ respectively. The calculated energy gap width and the ionisation energy were 0.43 eV and 0.15 eV, respectively. The variation in the charge carrier concentration versus temperature is discussed. The scattering mechanism was evaluated over the entire range of temperature. Additionally, other important parameters were estimated, such as the diffusion coefficient, the mean free time and the diffusion length of holes. These properties have not been reported to date.
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1. Introduction

In the past three decades, there have been significant research interest in chalcogenide materials because of the interesting physical properties of these materials and their wide technological applications[(1)]. There is increasing interest in ternary compound semiconductors with the general formula III-III-VI_2 because of their attractive physical properties, anisotropic, quasi-two-dimensional structure and unusual optical and photoelectric characteristics[(2)]. Ternary semiconductor compounds with the formula $TlAB_2$ (A: As, Sb, Bi and B: Te, Se, S) have been proposed for various application such as a coustoptic detectors, infrared detectors, thermoelectrics, and switching and memory elements[(3)]. Narrow-gap semiconductors have attracted considerable interest due to their wide application in infrared optoelectronics [(4)]. $TlBiTe_2$ is a narrow gap semiconductor [(5)], belonging to the family of III-V-VI ternary compounds of the general type $TlBiX_2$ (X = Te, Se, S) often referred to as pseudo-lead chalcogenides because of their close chemical relation to the PbTe, PbSe and PbS. $TlBiTe_2$ has been the subject of several studies because of their interesting features, but its use has been limited because TI and its compounds have to carefully handled[(6)]. Nevertheless, there are few studies on some of the transport properties of $TlBiTe_2$. In particular, no detailed study of the electrical conductivity and Hall coefficient over a wide range of temperature has been performed. The objective of this work was to grow $TlBiTe_2$ single crystals and to study the conductivity and Hall coefficient in these crystals. The properties of this compound have not been reported to date.

2- Experimental arrangement:

2-1- Growth technique.

Ingots of $TlBiTe_2$ were synthesized by direct fusion of stoichiometric amounts of spectroscopically standardised elements (Aldrich mart) with a purity of 99.999%. The samples were prepared by direct melting of the starting materials placed in quartz ampoules sealed under vacuum at approximately 10^{-6} Torr. The silica ampoule and its load was placed on a tray made from a heat-resistant alloy to minimise the effect of heat loss, for homogeneous distribution of heat and to protect the muffle furnace from the explosion hazard of the silica tube. The entire assembly was then placed in a controlled muffle furnace and the temperature raised gradually in 20ºC/h steps until the reaction occurred, as determined from previous studies [(7)]. At this point, the temperature was held constant for 10 hours, after which it was raised by 40ºC its rise is then continued to some 40°C above the melting point (520ºC) of the compound and held constant at this last stage for several hours. The sample was shaken several times to ensure complete mixing of the components. During this stage, any strain present in the matrix was relieved. To obtain a uniform composition of stoichiometric material, it was necessary to cool the mixture very slowly at a rate of 5ºC /h until it reached 150ºC, followed by rapid cooling to room temperature. These procedures take a long time to complete. The ingot obtained contained silvery, dark metallic crystals. X-ray diffraction of the synthesised crystals was performed using monochromatic Cu-Kα radiation.

The prepared material was highly crystalline, as determined by diffraction, and the diffraction data did not show the presence of any secondary phases.

2-2- Measurement technique:

To study the electrical conductivity and Hall effect, a rectangular sample was prepared. After polishing, the sample dimensions were 7.5 x 2 x 1 mm^3. The sample had a length three times its width. This aspect ratio is useful to avoid a Hall voltage drop. The electrical conductivity and Hall effect measurements were measured using a DC four probe method. The sample was placed in an evacuated pyrex cryostat[8]. The cryostat works as a liquid nitrogen container and is supported with electric heaters for low- and high-temperature measurements, respectively. The magnetic field value in the experiment was 0.5 T using a GMW electromagnet model 5403. The electrical conductivity and Hall coefficient were measured by a DC compensation method. Ohmic contact was made with the aid of silver paste. These contacts were ohmic in the range of the applied voltage. The ohmic nature of the contact was checked by recording the current-voltage characteristics. Details of the experimental procedures and apparatus have been published [9].

3- Results and Discussion:

Fig.1 shows the temperature dependence of the electrical conductivity σ for a $TlBiTe_2$ single crystal in a temperature range from 178 K to 568 K. The curve can be subdivided into three regions. The first region represents the extrinsic range. In this region, σ increases slowly with temperature, and the number of ionised acceptors mainly determines the carrier concentration. This effect occurs naturally as a result of the transition of carriers from the impurity level to the conduction band. The depth of the acceptor centre was determined from the region in which the conductivity is predominantly due to the impurity atoms and was found to be 0.16 eV. The second region represents the transition region (248 - 443 K), in which the behaviour of σ is governed by the behaviour of both the charge carrier concentration and their mobility. In this region, the increase in the electrical conductivity is due to the increase in mobility. The carrier density in this temperature regime remains practically constant until the intrinsic region is reached. Above 443 K, intrinsic conduction begins, and σ increases sharply. This finding reveals that both electrons and holes contribute to conduction at this high-temperature range. The dependence of this temperature follows the relation:

$$\sigma = \sigma_o \exp\left(-\frac{\Delta E_g}{2KT}\right) \qquad (1)$$

where σ_o is the pre – exponential factor and ΔEg is the width of the energy gap. Using this formula, the energy gap ΔEg is 0.43 eV. The value of σ at 300K is equal to 5.06 x 10^{-6} Ω^{-1} cm^{-1}.

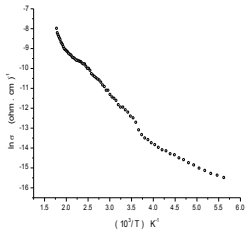

Fig. 1. Temperature dependence of the electrical conductivity

From the measurements of the Hall coefficient, it is evident that the sign of the Hall coefficient of $TlBiTe_2$ is positive over the entire range of investigation, indicating that the compound is a p-type semiconductor. The Hall coefficient at room temperature was 4.46 x 10^8 cm^3/C. The temperature dependence of the Hall coefficient for $TlBiTe_2$ specimen is shown in Fig. 2.

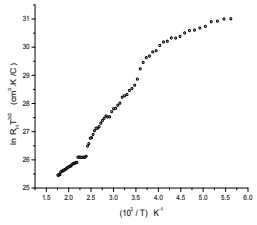

Fig.2. Temperature dependence of the Hall effect

Determination of the energy gap and ionisation energy from the Hall data is possible by plotting the relationship between Ln R_H $T^{3/2}$ and $10^3/T$ as shown in Fig. 3.

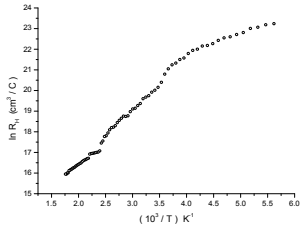

Fig. 3. Relationship between R_H $T^{3/2}$ and $10^3/T$

From this figure, three regions of the curve are also observed. This result agrees with that observed in Fig. 1. From the intrinsic region, ΔEg was found to be 0.43 eV, whereas in the extrinsic region, the value of ΔEa was estimated to be 0.15 eV. These data are approximately in good agreement with those obtained from the electrical conductivity data. A combination of the Hall measurements and electrical conductivity data were used to study the temperature dependence of the mobility of the charge carriers. Fig. 4 shows the variation of μ as a function of temperature. The variation of μ with temperature can be divided into two regions. At low temperature, μ increases with

increasing temperature with the following relation: $\mu \alpha T^{1.66}$. Such behaviour is characteristic of a scattering mechanism of charge carriers with ionisation impurities. In the high-temperature range, which is the intrinsic conduction region, the hole mobility decreases with increasing temperature according to the relation $\mu \alpha T^{-2}$, which indicates that the scattering mechanism in this temperature range is caused by acoustic lattice vibrations. The hole mobility at room temperature 2257.53 cm^2/ V sec. The charge carrier concentration was calculated from the Hall coefficient data using the relation:

$p = 1/R_H e$, where p is the hole concentration and e is the electron charge.

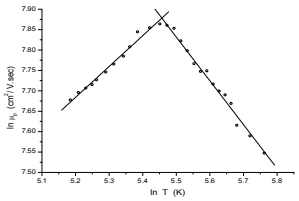

Fig. 4. Behaviour of the Hall Mobility as a function of temperature

The variation of the number of majority carriers versus reciprocal temperature is shown in Fig. 5. At room temperature, the concentration reaches a value of 1.4 x 10^{10} cm^{-3}. At low temperature (178 - 248 K) in $TlBiTe_2$, the carrier concentration is determined by the number of ionised acceptors. The variation of the carrier concentration is quite slow. Because the $TlBiTe_2$ sample exhibits intrinsic behaviour at temperatures above 443 K, the value for the intrinsic concentration will be given by:

$$P_i = 2\left(\frac{2\pi K}{h^2}\right)^{\frac{3}{2}} (m_n^* m_p^*)^{3/4} T^{3/2} \exp\left(-\frac{\Delta E_g}{2KT}\right) \quad (2)$$

where symbol have their usual meaning, and the energy gap width determined from this relation is 0.43 eV.

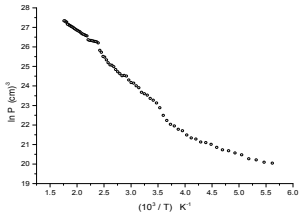

Fig. 5. Variation of carrier concentration with temperature

Calculating the diffusion coefficient for holes yielded a value of 58.47 cm^2/sec. Assuming the effective mass for holes is equal to the rest mass, and using the value for the hole mobility at room temperature, the mean free time could be determined and was equal to 1.393 x 10^{-12} sec. Additionally, the diffusion length of holes in the $TlBiTe_2$ specimen was 9.024 x 10^{-6} cm.

4- Conclusion:

The preparation and electrical properties of Thallium Bismuth ditelluride single crystals is reported in the present work. Measurements of the electrical conductivity and Hall coefficient were performed over a temperature range from 178 - 568 K. All measurements were performed under vacuum in a special cryostat designed for this purpose. The measured Hall coefficient indicates p-type conductivity for our sample with a hole concentration of 1.4 x 10^{10} cm^{-3} at room temperature. The conductivity and Hall mobility at 300 K were 5.06 x 10^{-6} Ω^{-1} cm^{-1} and 2257.53 cm^2/V.sec, respectively. The scattering mechanism was evaluated over the whole temperature range and was found to be due to charge carriers with ionised impurities at low temperature and to lattice scattering in the high temperature regime. The width of the band gap was estimated to be 0.43 eV. The position of the acceptor level was determined to be at 0.15 eV. The diffusion coefficient, mean free time and the diffusion length of holes were also evaluated.

Corresponding author:
F. S. Bahabri
Physics Department, Science of Faculty for Girls, King Abdul Aziz University- KSA
f_s_bahabri@hotmail.com

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