

## Thermal Transport Properties of TlInTe<sub>2</sub> Single Crystals

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*Abstract.* Thallium indium ditelluride single crystal, was prepared by a special design constructed by our group. A brass working chamber designed for measuring (TEP) in a wide range of temperature was used. The experimental results indicates that TlInTe<sub>2</sub> is of p-type conductivity. The mobility of charge carriers, holes and electrons was found to be  $2.129 \times 10^3 \text{ cm}^2 / V, \text{ sec}$  and  $1.218 \times 10^5 \text{ cm}^2 / V, \text{ sec}$  respectively. The effective masses of the majority and minority carriers were deduced to be  $5.367 \times 10^{-37} \text{ kg}$  and  $6.856 \times 10^{-43} \text{ kg}$  respectively. The diffusion coefficient, relaxation time and diffusion length for holes was calculated to be  $551.436 \text{ cm}^2 / \text{sec}$ ,  $7.142 \times 10^{-21} \text{ sec}$  and  $1.986 \times 10^{-9} \text{ cm}$  respectively. Also  $D_n, \tau_n, L_n$  for the electrons was calculated to be  $3.156 \times 10^3 \text{ cm}^2 / \text{sec}$ ,  $5.222 \times 10^{-26} \text{ sec}$  and  $1.284 \times 10^{-11} \text{ cm}$  respectively. In addition to these pronounced parameters, the efficiency of the thermoelectric element (figure of merit) was evaluated, which leads to better application in many fields .

*Keywords:* TlInTe<sub>2</sub>, single crystals, thermoelectric power, semiconductor, charge carriers.

### 1. Introduction

Most of the technological, electronic and opto-electronic applications utilize semiconductor materials in crystalline forms. The discovery of new semiconductor materials on the basis of  $A^{\text{III}}B^{\text{III}}C_2^{\text{V}}^{\text{III}}$  is an urgent problem due to the reliability of these compounds in solid-state electronic. TlInTe<sub>2</sub> belongs to the family<sup>[1]</sup> TlAX<sub>2</sub> (A: In, Ga; X: S, Se,

Te). It forms a tetragonal lattice of group symmetry  $D_{4h}^{18} - 14/mcm$ . Therefore it is structurally analogous to TlSe. In  $TlInTe_2$  four Te atoms forms a tetrahedron with a strongly bound  $In^{+3}$ -ion in its centre. These tetrahedral form covalent  $[In^{3+}Te_2^{2-}]^{-1}$  chains parallel to the C-axis of the crystal. They are bonds to each other by Octahedrally arranged  $Tl^{1+}$ -ions by means of weak ionic bonds. The resulting lattice exhibits a one-dimensional organization, which is responsible for the fibrous structure of the material. Numerous studies determined physical and crystallographic data such as melting point, density, form and size of the crystal cell, infrared spectra and nonlinear electrical behavior<sup>[2-7]</sup>. Other investigators analyzed properties of electronic band structure, dielectric function, energy gaps, positions of acceptor levels and carrier concentration<sup>[8-12]</sup>.  $A^{III}B^{III}C_2^{VI}$  compounds are formed in the layered-chain structure as  $A^{III}C^{VI} - B^{III}C^{VI}$  in which the components  $A^{III}C^{VI}$  and  $B^{III}C^{VI}$ <sup>[13]</sup> have the ratio 1:1. For instance, for the compounds  $TlInTe_2$ , the components are arranged in the form  $TlTe-InTe$  and they are called the ternary-chain  $TlInTe_2$  type. Thermal transport properties of  $TlInTe_2$  single crystals are not well known. Also as far as we know; the published literature is still insufficient to throw a clear light upon the actual behavior of this compound. In view of this, the present work aims to prepare and investigate the thermoelectric power of the  $TlInTe_2$  single crystal, since there is no information about these properties for  $TlInTe_2$  in the literature. Moreover, the thermoelectric measurements for this material, give the chance of practical application especially in the field of energy conversion.

## 2. Experimental Procedure

The samples we have worked with were  $TlInTe_2$  single crystals. They have been grown from melt by the modified Bridgman technique. The purity of the materials used was as follows Tl, 99.9999%, In, 99.9999% and Te, 99.9999%. Stoichiometric mixture of the elements was used as starting material in the growth experiments. At the beginning of the growth run, the ampoule with its charge was held in the hot zone of the furnace at 1137K for 10 h. For melt homogenization, the charge was shaken during heating several times to accelerate the diffusion of contaminates through each other. Then the

ampoule was moved into the middle zone of the furnace with a temperature of 1045K according to the phase diagram<sup>[14]</sup> at rate of 2.5 mm/h. Afterwards, the ampoule was cooled down slowly in the third zone of the furnace, then the furnace was switched. Details of the experimental equipment for crystal growth and of preparation procedures are described elsewhere<sup>[15]</sup>.

The thermoelectric power (TEP) of bulk specimen at different temperature was measured. The used sample holder was of pressure contact type. A vacuum working chamber was locally constructed for the present work and was designed<sup>[16-17]</sup>, in a way that, it allows measurements at a wide range of temperature. In this work, a compensation method is used for measuring voltages without drawing an appreciable current using a tensely potentiometer type (UJ33E). The potentiometer is used for measuring the thermo-e.m.f., while  $T_1$  and  $T_2$  are measured using digital multimeter model HC-5010.

The thermoelectric power of the investigated  $TlInTe_2$  is measured through out a temperature range from 158-448K. A temperature gradient exists along the crystal when an average temperature difference between the ends of the specimen is kept small (not greater than 5°C in our range of temperature). More details about the apparatus and technique of measuring have been published<sup>[18]</sup>.

### 3. Results and Discussion

The results of the temperature dependence of thermoelectric power (TEP) of  $TlInTe_2$  single crystals are given in Fig. 1. The results and figure indicate the following points: 1) Our sample shows p-type conductivity within the temperature range of investigation, which is in quantitative agreement with our previous data<sup>[12]</sup> of the hall coefficient, 2) the room temperature TEP value for  $TlInTe_2$  mounted to  $2.2 \mu V \text{ deg}^{-1}$ , 3) the figure shows that the value of the thermoelectric power decreases as the temperature rises. This may be due to the presence of some crystal defects or trapping centers in the direction of the carrier flow, 4) with further rise of temperature,  $\alpha$  increases rapidly till reaching its maximum value ( $100 \mu V / \text{deg}$ ) corresponding to 240K. Such behavior led to the assumption that, more holes are generated and contribute to the increment of ( $\alpha$ ) values as the temperature rises, 5) a third region in the

same figure is observed where  $(\alpha)$  rapidly falls above 240. The decrease of  $(\alpha)$  magnitude is regarded as a result of the compensation process which takes place in this temperature range, 6) with further rise of the temperature,  $\alpha$  increases very rapidly. Such behavior is expected in this intrinsic range where generation of both carriers (electron and holes) contributes to the increment of  $(\alpha)$  value. As follows from the expression the EMF of a semiconductor in the intrinsic region is given by<sup>[19]</sup>:

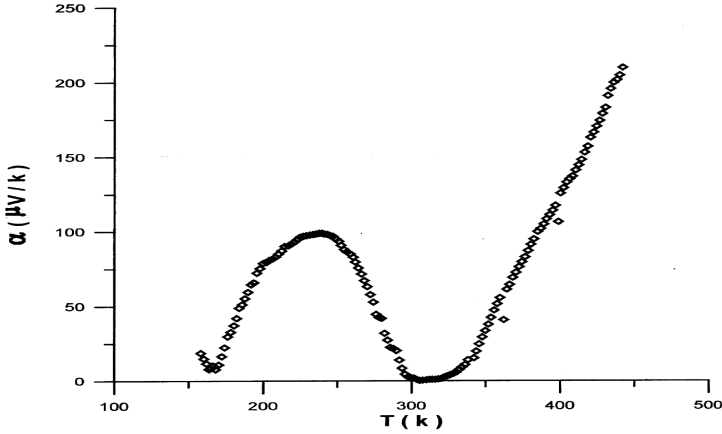


Fig. 1. Relation between thermoelectric power and temperature for  $TlInTe_2$  single crystals.

$$\alpha = -\frac{k}{e} \left[ \frac{\mu_n - \mu_p}{\mu_n + \mu_p} \left( \frac{\Delta E_g}{2kt} + 2 \right) + \frac{3}{4} \ln \frac{m_n^*}{m_p^*} \right]$$

Where  $\mu_n$  and  $\mu_p$  are the electron and hole nobilities,  $m_n^*$  and  $m_p^*$  are the effective masses, and  $\Delta E_g$  is the width of the forbidden band. This formula predicts that a plot of  $\alpha$  as function of the reciprocal of the temperature, in the intrinsic range, should be a straight line with parameters determined by  $b = (\mu_n/\mu_p)$  and  $(m_n^*/m_p^*)$ . Figure 2 shows a plot of  $\alpha$  versus  $10^3 T^{-1}$  for p-type  $TlInTe_2$ . This linear relation has negative slope, indicating the increase of  $\alpha$  with elevating surrounding temperature. Knowing  $\Delta E_g$  from the Hall<sup>(12)</sup> data and assuming  $(m_n^*/m_p^*)$  that does not vary with temperature, it was found that  $(\mu_n/\mu_p) = 5.7245$ . Thus, by using  $\mu_p = 2.1291 \times 10^4 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$  at room temperature, then  $\mu_n = 1.2188 \times 10^5 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ . Measurements of the temperature dependence of the electrical conductivity the Hall<sup>(12)</sup> coefficient and

thermo-EMF enabled us to find the mean effective masses of the electrons and holes. Their ratio was evaluated to be  $(m_n^*/m_p^*)=1.278 \times 10^{-6}$  from the intercept of the curve. This means that the effective mass of a hole is greater than that of an electron.

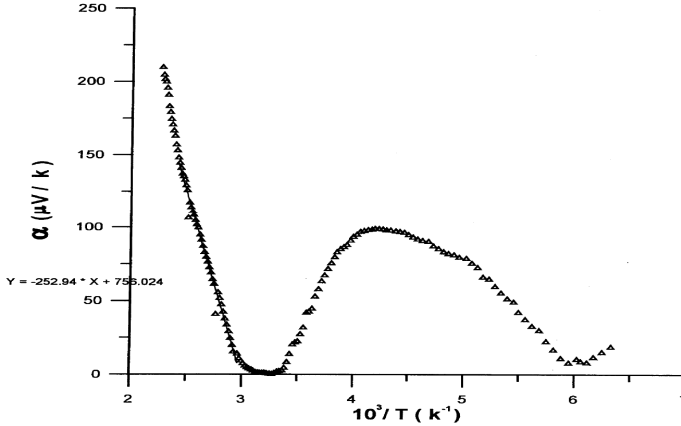


Fig. 2. The relation between  $\alpha$  and  $10^3/T$  for TlInTe<sub>2</sub> single crystal.

Another important relation was suggested for application in the extrinsic region<sup>(20)</sup>:

$$\alpha = \frac{k}{e} \left( 2 - \ln \frac{ph^3}{2(2\pi m_p^* kT)^{3/2}} \right)$$

Plotting the above relation between  $\alpha$  and  $\ln T$  we obtain Fig. 3. This figure shows that  $\alpha$  decreases linearly with the increase of temperature in the temperature, corresponding to the extrinsic conductivity region. Thus the effective mass of holes was evaluated to be  $5.367 \times 10^{-37}$  kg. Combining the value with the above mentioned results for the ratio  $(m_n^*/m_p^*)$ , one obtains an effective mass of minority carriers of the value  $m_n^* = 6.856 \times 10^{-43}$  kg. Using the effective mass values of electrons and holes, the relaxation time for both current carriers can be determined. Its value for holes comes to be  $7.142 \times 10^{-21}$  s, whereas for the electrons it equals  $5.222 \times 10^{-26}$  s. The diffusion constant is related to the mobility of charge carriers; its value for holes and electrons can be deduced as  $D_p = 551.44 \times 10^3 \text{ cm}^2 \text{ s}^{-1}$ ,  $D_n = 3.156 \times 10^3 \text{ cm}^2 \text{ s}^{-1}$  respectively. The diffusion coefficient as noticed is inversely proportional to the effective mass of holes and electrons. The electron mobility as calculated is much higher

than the hole mobility, this result is acceptable since the hole effective mass is greater than that of the electrons. Combining the values of diffusion coefficient and relaxation time, one can obtain the diffusion length of free carriers  $L_p = 1.984 \times 10^{-9}$  cm and  $L_n = 1.284 \times 10^{-11}$  cm for holes and electrons respectively. Figure 4 represents the dependence of TEP on the carrier density; it is shown that  $\alpha$  increases sharply with the carrier concentration. The same behavior is observed when we plot  $\alpha$  versus  $\ln\sigma$  for  $TlInTe_2$  sample as shown in Fig. 5. It seems that TEP increases with the electric conductivity. The increase in the value of  $\alpha$  with concentration can be attributed to, as the temperature increase, the carrier density increase and the rate of diffusion of charge carrier's increase, this leads to increase of  $\alpha$  with carriers concentration and conductivity. The choice of materials for thermocouples, thermoelectric generation and refrigerators is based on the efficiency parameter  $Z$ , defined by the relation  $Z = (\alpha^2\sigma/k)$ . However the term figure of merit is a measure of both performance and efficiency of a certain thermoelectric element. For our best  $TlInTe_2$  samples the obtained value of  $Z$  permits the practical application as thermoelectric element. The proposed treatment of the experimental data sheds new light on the main physical parameters in  $TlInTe_2$  single crystals. However, those parameters are found to be sufficient to give complete information about the general behavior of the  $TlInTe_2$  crystal. This gives the chance of practical application especially in field of energy conversion.

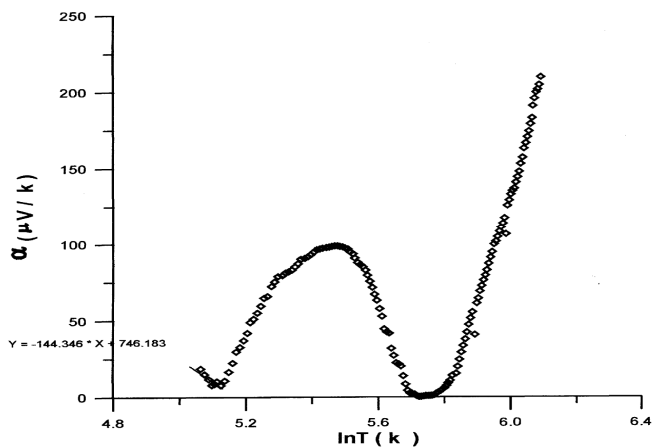


Fig. 3. Plot of  $\alpha$  against  $\ln T$  for  $TlInTe_2$  single crystal.

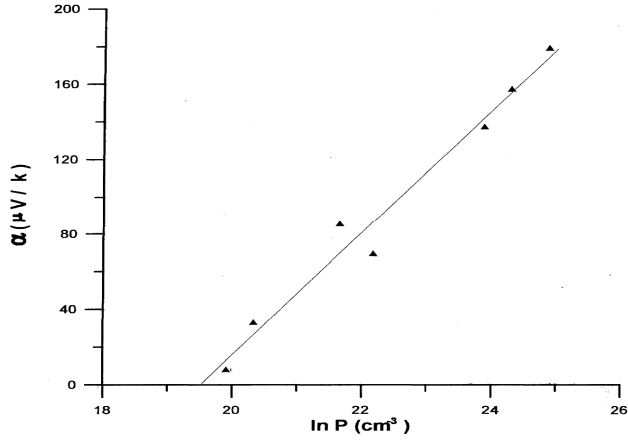


Fig. 4. The dependence representation of the TEP and concentration of carriers for  $TlInTe_2$  single crystal.

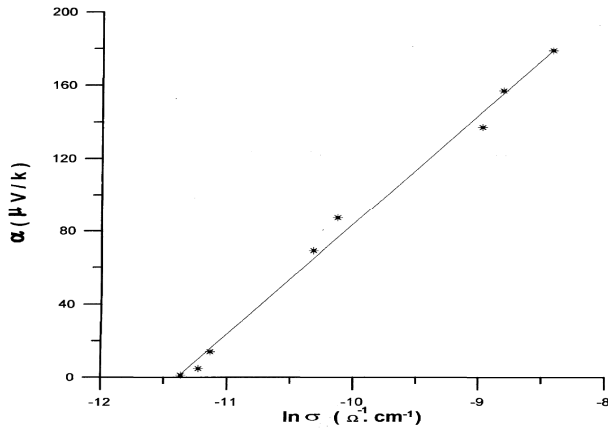


Fig. 5. Illustrate TEP variations with the conductivity for  $TlInTe_2$  single crystal.

#### 4. Conclusion

In the present paper, measurements of thermoelectric power in a wide range of temperature for  $TlInTe_2$  single crystal were reported. The experimental data, give us the chance to determine the following pronounced parameters; conductivity type carriers, mobility, effective masses of charge carriers, diffusive coefficient and diffusive length as

well as the relaxation time of both types of charge carriers. This mode of investigation (crystal growth and thermoelectric properties study) is an ideal way for finding out the possibility of making applications for these semiconductor compounds especially in the field of energy conversion, semiconductor devices and electronic engineering.

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## خواص الانتقال الحراري لبلورات أحادية المركب ثاليوم - إنديوم - ثنائي التليريوم

أحمد الغامدي، و نجات توفيق\*، و فرج الحازمي، و صالح الحنيطي

و سميرة القحطاني\*، و فتحية شكر\*

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الملك عبدالعزيز - جدة - المملكة العربية السعودية

المستخلص. تم استخدام التصميم الخاص المميز للإنماء البلوري من المصهور، اعتمادًا على تقنية بريجمان في تنمية المركب الثلاثي الشالكوجنيدي ثاليوم- إنديوم - ثنائي التليريوم، والذي تم تنفيذه بالإمكانات المحلية، دون الاستعانة بمحركات بطيئة السرعة. كما تم تصميم خاص لغرفة التشغيل النحاسية المستخدمة لدراسة ظاهرة القدرة الكهروحرارية، والتي تسمح لنا بإجراء القياسات تحت تبريد مناسب في مدى واسع من درجات الحرارة. أظهرت نتائج القياس أن موصلية شبه الموصل من النوع الموجب، وأمكن تعيين انسيابية حوامل التيار الحرة للثقوب والإلكترونات، ووجدت تساوي:

$$16^3 \text{ cm}^2 \text{ N sec} \times 2.129 \text{ و } 16^5 \text{ cm}^5 \text{ V sec} \times 1.218$$

على الترتيب. كما أمكن تعيين الكتلة الفعالة لحوامل التيار السائدة والأقلية، ووجدت تساوي:

$$10^{-37} \text{ kg} \times 5.367 \text{ و } 10^{-43} \times 6.856$$

على التوالي. أمكن تقدير معامل الانتشار، وزمن الاسترخاء، وطول مسار الانتشار للفجوات وهي كالتالي:

$$551.436 \text{ Cm}^2/\text{Sec} \text{ و } 10^{-21} \times 7.142 \text{ و } 10^{-9} \times 1.984$$

أما بالنسبة للإلكترونات، فحسبت أيضًا قيم  $D_n$  ،  $\tau_n$  ،  $L_n$  على الترتيب كالتالي:

$$3.156 \times 10^3 \text{ cm}^2/\text{Sec} \text{ و } 5.222 \times 10^{-26} \text{ و } 1.284 \times 10^{-11} \text{ Ca}$$

بالإضافة إلى ذلك، كفاءة العنصر الكهروحراري (معامل الاستحقاق الكهروحراري) أمكن إيجاد قيمته وهي:

$$Z=8.43 \times 10^{-9} \text{ K}^{-1}$$