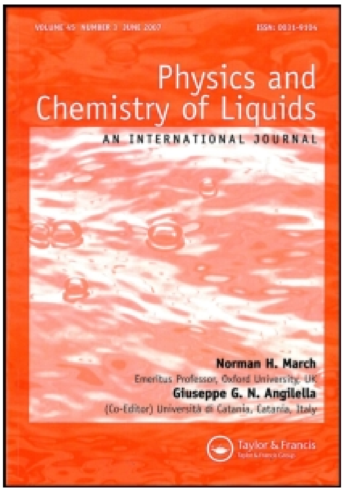

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Electrical and Thermoelectric Properties of $CuInTe_2$ in the Solid and Liquid Phases

N. H. Mousa[a]; M. M. El-bahay[a]; A. Abdelghany[a]; A. H. Abou El Ela[a]
[a] Physics Department, Faculty of Science Al-Azhar, University for Girls, Nasr City, Cairo, Egypt

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ELECTRICAL AND THERMOELECTRIC PROPERTIES OF $CuInTe_2$ IN THE SOLID AND LIQUID PHASES

N. H. MOUSA, M. M. EL-BAHAY, A. ABDELGHANY and A. H. ABOU EL ELA

Physics Department, Faculty of Science Al-Azhar University for Girls, Nasr City, Cairo, Egypt

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Measurements of the electrical conductivity and thermoelectric power of $CuInTe_2$ in the temperature range from 400°C to 970°C shows that the thermoelectric power changes sign from positive in the solid state to negative in the liquid state above its melting point. The experimental data were explained on the basis of a model developed for the density of states and electrical transport in solid amorphous semiconductors [1]. The activation energy from electrical conductivity was found to be 0.31 ev for the solid and 0.79 ev for the liquid and the coefficient of the linear decrease of the energy gap with temperature was found to be 1.18×10^{-4} ev/°K.

Keywords: Electrical conductivity; thermo electric power; energy gap

INTRODUCTION

Much research and attention have been devoted to understand the properties of amorphous and liquid semiconductors. Various models were suggested for liquid semiconductors, and the most comprehensive attack to the theoretical problems has been made by Mott [2, 3] and Cutler [4]. Ternary chalcopyrite semiconductors have recently attracted attention because of their possible applications in electro-optical devices. High efficiency solar cells are often fabricated using these ternary compounds [5–7].

The aim of the present paper, is to study the electrical conductivity and thermoelectric power of $CuInTe_2$ semiconductor in a wide range of temperatures in the solid and liquid states. $CuInTe_2$ is a direct energy gap semiconductor, its melting point is 780°C and crystallizes in the chalcopyrite structure.

EXPERIMENTAL

The samples were prepared by melting the proper amounts of high purity component elements (99.999%) taken in their stoichiometric ratios. The material was sealed in a silica tube at 10^{-3} Pa, and heated at 1200°C for 12 h with frequent rocking using an oscillating oven to ensure homogeneity of the melt. Then the tube was quenched to room temperature. The solid material is then heated in an inert atmosphere until it melts and then transferred to the measuring cell.

Measurements of the electrical conductivity and thermoelectric power were carried out in the measuring cell which was fitted with graphite electrodes, heaters, and thermocouples for accurate measurements of temperature up to 0.2°C [8]. A highly stabilized power supply, a sensitive voltmeter, and a sensitive digital electronic multimeter capable of measuring currents as low as 10^{-6} A were used. The sample was investigated up to 200°C above its melting point.

RESULTS

X-ray diffraction techniques have been applied to study the structure of $CuInTe_2$ ternary compound. Figure 1 shows x-ray diffraction patterns obtained for the bulk material, it is clear that no evidence for the existence of more than one phase [9, 10] was observed. The peak heights and positions are in good agreement with the data reported for the bulk material [11, 12].

Figure 2 shows the temperature dependence of the electrical conductivity in the solid and liquid states. It is divided into two parts, the first one for solid and the second for liquid. Both of them increases exponentially with increasing the temperature, between them there is a decrease of the electrical conductivity from 636°C till it reaches the melting point of the compound 780°C. In the solid state the activation energy is $E_{\mathrm{solid}} = 0.31$ ev, while at higher temperatures in the liquid state the activation energy is $E_{\mathrm{liquid}} = 0.79$ ev.

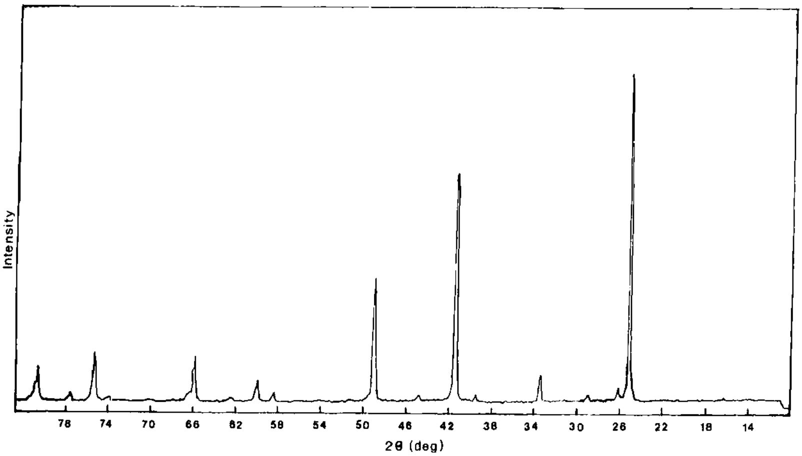

FIGURE 1 X-ray diffraction pattern of $CuInTe_2$ (Powder Sample).

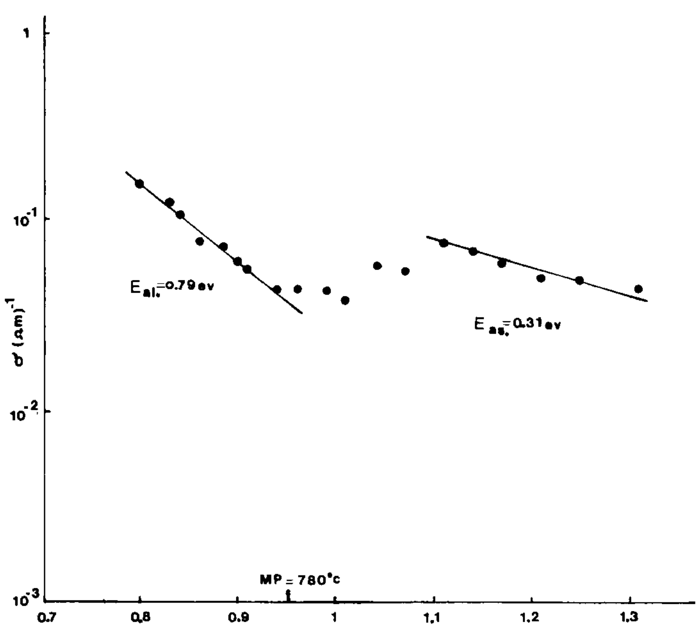

FIGURE 2 Temperature dependence of the electrical conductivity of $CuInTe_2$ in solid and liquid states.

Figure 3 shows the temperature dependence of the thermoelectric-power in the solid and liquid states. It is observed that the thermoelectric power is positive in the range from 460°C to 700°C, at 735°C it begins to change its polarity and become negative.

DISCUSSION

From Figure 2 the activation energy of $CuInTe_2$ in the solid phase equal to 0.31 ev which may be attributed to impurity conduction. At the melting point the electrical conductivity decrease which may be attributed to changes in the short range order on melting and the subsequent decrease in carrier mobility. In the liquid state ln σ increases linearly with temperature, with an activation energy equal to 0.79 ev which indicates a weakening of the influence of impurities and a change from extrinsic conduction to intrinsic conduction in the liquid state.

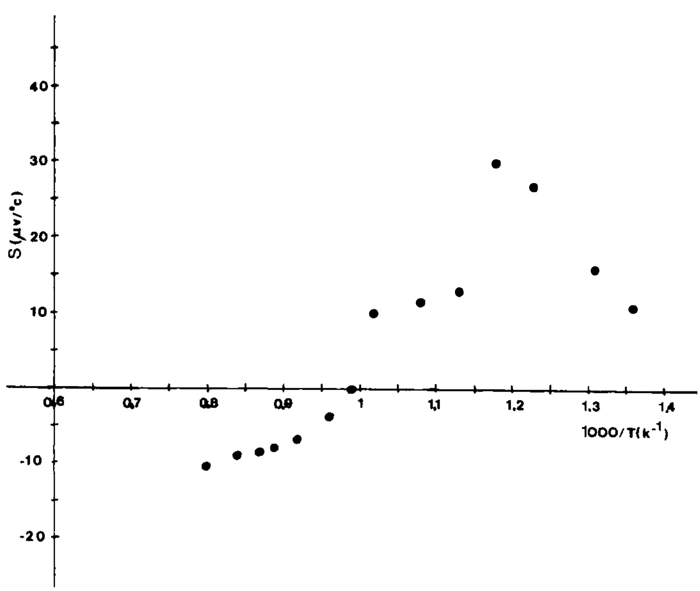

FIGURE 3 Temperature dependence of the thermoelectric power of $CuInTe_2$ in solid and liquid states.

Figure 3 shows the temperature dependence of the thermoelectric power S. Positive S indicates large predominance of holes in the electrical transport and the rapid decrease of S with temperature in the solid state just before melting may be attributed to variation in the short range order during softning and melting, and the resulting variation in the width of conduction and valence bands which affects the magnitude of the thermoelectric power. At the melting point, a sudden decrease in the thermoelectric power and σ is observed, which may be attributed to changes in the short range order and the decrease in carrier mobility. The values of the activation energy 0.31 ev suggest that the conductivity is attributed to extended states in the conduction and valence bands.

Above the melting point and in the liquid state S becomes negative. It appears that $CuInTe_2$ behaves in the liquid state as n-type semiconductor. Moreover, inversion of sign of S occurs where σ decreases and becomes minimum. This inversion can be understood in terms of transition between transport in two different bands. The region between the peaks in magnitude of S is explained by ambipolar transport which suggests that there is cancellation between the positive and negative contributions to the thermoelectric power due to hole and electron transport.

The electrical conductivity is determined from

$$\sigma = \sigma_0 \exp\left(- \frac{E_f - E_v}{KT} \right) \tag{1}$$

The value of the constant σ_0 various strongly with the conduction process. $(E_f - E_v)$ depends on temperature and is given by:

$$E_f - E_v = E(0) - \gamma T \tag{2}$$

Thus

$$\sigma = \sigma_0 \exp(\gamma / K) \ \exp[-E(\mathrm{o}) / KT] \tag{3}$$

The temperature coefficient γ can be calculated directly from the thermoelectric power equation which is expressed as

$$S = \frac{k}{e}\left(\frac{E(o)}{KT} - \frac{\gamma}{k} + A\right) \tag{4}$$

where the constant A is related to scattering mechanisms. If A is known, γ can be determined directly from the intercept on the $1/T = o$ axis of a plot of S vs $1/T$. By combining (1) and (4), we obtain the relation between σ and S.

$$\sigma = \sigma_0 \exp\left(-e\frac{S}{k} + A\right) \tag{5}$$

Figure 3 shows that the relation between S and $1/T$, above the melting point in the liquid state, is a straight line. The extrapolation of this line to the axis $1/T = o$ yields: $\gamma/k = -e/k\ S_o + A$

For $A \geqslant o$, $\gamma/k \geqslant S_o/86$. According to Culter and Mott [13], the constant A is of order unity for disordered structures. A recent investigation of the thermoelectric power of amorphous chalcogenides [14] suggests that A may be larger than unity for highly disordered materials. In our discussion, we assume that $A = 1$, and the extrapolation of the curve gives for the coefficient γ a value 1.18×10^{-4} ev/°k. The obtained value of γ indicates that the temperature dependence of the gap for liquid $CuInTe_2$ is of the same order as that found for liquid Te-Se alloys [15]. It seams likely that the large linear decrease of the gap with increasing temperature is related to that the difference between the distances from one atom to nearest and next-nearest neighbours decrease [1].

Various workers [13, 16, 17] have attributed the negative values of S to a large predominance of electrons in electrical transport. The equations of the electrical conductivity and thermoelectric power for liquid semiconductor can be written as:

$$\sigma = \sigma_e + \sigma_h = ne\mu_e + pe\mu_h$$

where n and p are the concentrations of electrons and holes, μ_e and μ_h the mobilities of electrons and holes, σ_h, σ_e are the hole and electron conductivities and the thermoelectric power is given by:

$$S = \frac{-\frac{k}{e}\int \sigma(E)\left[\frac{E-E_f}{KT}\right]\left(\frac{\partial f}{\partial E}\right)dE}{\int \sigma(E)\left(\frac{\partial f}{\partial E}\right)dE}$$

Dutchak [18] had shown that the thermoelectric power for bipolar transport can be written as:

$$S = -\left(\frac{k}{e}\right)\left[\frac{Eg}{2KT}\right]\left[\frac{\sigma_e - \sigma_h}{\sigma_e + \sigma_h}\right] \tag{6}$$

where Eg is the energy gap.

It is clear from Eq. (6) that the thermoelectric power depends on the difference between σ_e and σ_h and varies strongly as σ_e and σ_h vary with temperature. Positive S in the solid state indicates that $\sigma_h > \sigma_e$ due to high density of holes or high hole mobility. In the liquid state σ_e becomes larger than σ_h and S changes sign and becomes negative.

CONCLUSION

$CuInTe_2$ behaves as n-type semiconductor in the liquid state. The inversion from P-type in the solid phase to n-type can be understood in terms of transition between transport in two different bands. The electrical conduction in liquid $CuInTe_2$ could be analyzed by the model developed by Mott. The electrical conduction mechanism is due to holes excited into extended states near the band edge, and the energy gap is 1.58 ev. The temperature coefficient γ is found to be 1.18×10^{-4} ev/°K which shows a large decrease of the gap with temperature.

References

[1] Mott, N. F. (1970). *Philos. Mag.*, **22**, 7, *Philos. Mag.*, **24**, 1.
[2] Mott, N. F. (1966).*Phil. Mag.*L3, *Ibid.*, **24**, 1, 1971.
[3] Mott, N. F. (1967). *Adv. Phys.*, **16**, 49.
[4] Cutler, M. (1977). Liquid Semiconductors, Academic Press, New York.
[5] Neumann, H., Hoerig, W., Savel'ev, V., Legzdonis, L., Shuman, B. and Kuehn, G. (1981). "Thin Solid Films", **79**, 167.

[6] Neumann, H. in "Optoelectronic materials and devices " edited by M. A. Hermann (PMN Polish Scientific, Warsaw, 1953).
[7] Kasmerski, L. L. (1977). *J. Phys. C.* **10**.
[8] Abou El Ela, A. H. and Abdelmohsen, N. (1982). *App. Phys. A.*, **29**, 39.
[9] Palatnik, L. S. and Rogacheva, E. I. (1967). *Sov. Phys. Dokl.*, **12**, 503.
[10] Zalar, S. M. (1966). J. Electrochem. Soc. **113**, 230.
[11] Kasmerski, L. L., Ayyagari, M. S., Sanborn, G. A., White, F. R. and Merrill, A. G. (1976). 'Thin Solid Films', **37**, 323.
[12] Abo El Soud, A. M., Hendia, T. A., Soliman, L. I., Zayed, H. A. and Kenawy, M. A. (1993). *J. Mater. Sci.*, 1182–1188.
[13] Cutler, M. and Mott, N. F. (1969). *Phys. Rev.* **181**, 1336
[14] Rockstad, K., Flasck, R. and Iwasa, S. (1972). *J. Non-Cryst. Solids.*, **326**, 8–10.
[15] Perron, J. C. (1972). *J. Non-Cryst. Solids.*, **272**, 8–10.
[16] Gobrecht, H., Mahdjuri, F. and Gawlik, D. (1971). *J. Phys. G.* 4, 2247.
[17] Labib, H., Fornazero. J. and Mesnard, G. (1978). *Phy. Chem. Liquid.*, **7**, 1.
[18] Dutchak, Ya.I., Kigus, I. P., Prokherenko, Ya. (1969). *Phys. Status Solidi* **31**, 25.