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Physical Characterization of Solid Solution $CdSe_xTe_{1-x}$ and its Solar Cell Applications.

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Electrical conductivity and dielectric properties of Bulk $CdSe_xTe_{1-x}$ ($0 \leq x \leq 0.4$).

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Abstract

Measurements of the dc, ac conductivity and the dielectric properties were made for polycrystalline $CdSe_xTe_{1-x}$ ($0 \leq x \leq 0.4$) at various frequencies (0.1-100kHz) and at various temperatures (293 - 413 K). The temperature dependence of the dc conductivity was measured in the temperature range (293-413K). It was found that the obtained dc activation energy for the investigated compositions decreases with the increase of Se content. The ac conductivity is found to be frequency and temperature dependent and obeys the $A\omega^s$ law where s decreases with the increase of temperature. The dielectric constant ε_1 and dielectric loss ε_2 decreased with the increase of frequency and increased with the increase of temperature as well as the increase of Se content. The ac conductivity and dielectric properties of these compositions are explained on the basis of the correlated barrier hopping model.

1.Introduction

$CdSe_xTe_{1-x}$ is a ternary II-VI semiconductor of the equivalent two binary compounds CdSe and CdTe. They have extensive applications in solar cells[1], transistors[2], photoconductors[3]. The interaction between CdSe and CdTe are formed within two wide concentration regions, one with CdTe base and hence with zinc blende structure (α-phase solid solution) and the other with a CdSe base and hence with the wurtizite structure (β-phase solid solution). Both regions are separated by a narrow ($\alpha+\beta$) phase zone which exists as a result of structural transformation from zinc blende to wurtizite structure[4]

Some of the published data on dc electrical conductivity mechanisms of these materials are in variance [5 -12]. No data concerning ac conductivity and dielectric properties are available in literature. In this paper, the dc, ac conductivity and dielectric properties of $CdSe_xTe_{1-x}$ ($0 \leq x \leq .4$) are studied in the temperature range (293 - 413 K) and in the frequency range (0.1-100 kHz). In a previous study[13], X-ray diffraction of $CdSe_xTe_{1-x}$ ($0 \leq x \leq .4$) showed that they have cubic polycrystalline structure. Linear variation of the lattice constant (a) with mole fraction x satisfies Vegard's law as:-

$a_{powder} = 6.478 \pm 9.12 \times 10^{-4} - (0.495 \pm 0.0037)x$.

Measurements of ac conductivity of chalcogenide semiconductors are used to understand the conduction process in these materials. Quantum-mechanical tunneling model QMT [14,15], overlapping–large polaron tunneling OLPT model [16], and correlated barrier hopping CBH model [17-19] are proposed to explain the ac conduction mechanism for different materials. Our results were discussed with respect to these models for conduction process.

2. Experimental Techniques.

$CdSe_xTe_{1-x}$ ($0 \leq x \leq .4$) compositions were prepared in bulk form as mentioned previously[13]. A digital Keithely (E 617A) electrometer was used to measure dc electrical resistance R_{dc} directly. The dc conductivity σ_{dc} was calculated from the equation $\sigma_{dc} = d/R_{dc}A$, where d is the thickness and A is the cross section area. A programable automatic RLC bridge (PM 6304 Philips) was used to measure the impedance Z, the capacitance C and the loss tangent $\tan \delta$ directly as a function of frequency in the range (0.1-100kHz). All investigated samples are represented on the screen of the bridge by a resistance R connected in

parallel with a capacitance C. The total conductivity was calculated from the equation: $\sigma_t(\omega) = d/Z\ A$. The dielectric constant was calculated from the equation: $\varepsilon_1 = dC/A\varepsilon_o$, where ε_o is the permittivity of the free space. The dielectric loss ε_2 was calculated from the equation: $\varepsilon_2 = \varepsilon_1 \tan\delta$, where ($\delta = 90 - \phi$), ϕ is the phase angle. All measurements are studied in the temperature range (293-413K) using a digital multimeter (Protec 81) provided by a chromel –allumel thermocouple adjacent to the sample.

3.Results and Discussion

3.1. Temperature dependence of the dc conductivity

The temperature dependence of the dc electrical conductivity for $CdSe_xTe_{1-x}$ ($0 \le x \le .4$) is shown in Fig.(1). It is indicated from the figure that σ_{dc} increases with temperature according to the equation:-

$$\sigma_{dc} = \sigma_0 \exp(-\Delta E/kT) \qquad (1)$$

where σ_0 is constant , k is the Boltzmann constant and ΔE is **the** dc conduction activation energy. Values of ΔE were calculated from the slopes of the obtained straight lines indicating one conduction mechanism in the whole studied range of temperature. Fig. (2) represents the variation of ΔE and room temperature dc conductivity $RT\ \sigma_{dc}$ with molar fraction x. it is indicated that ΔE decreases while $RT\ \sigma_{dc}$ increases with the increase of x. These results agree with Balyaev et al.[10] and Uthanna et al.[9]in their studies of dc conductivity for the investigated compositions. Balyaev et al.[10] showed that activation energy, as well as, resistivity decreases with the increase of x. Uthanna et al.[9] found that resistivity decreases exponentially with increasing x. According to Balyaev et al.[7,10] $CdSe_xTe_{1-x}$ ($0 \le x \le 0.4$) are inhomogeneous semiconductors with deep impurity level possessing large values of potential relief inhomogenety. They exhibit an impurity band with high

conductivity whose amplitude of potential relief inhomogenety is considerably lower than that of intrinsic zone. The activation energy is then expected to be less than half of the optical energy gap as in intrinsic semiconductors. The obtained values of ΔE and the values of E_g^{opt} obtained previously [13] are given in table (1) which indicate that ΔE is more less than ½ E_g for all compositions in the considered range. This is in agreement with the data of Balyaev et al[7,10].

3.2. Frequency and temperature dependence of ac conductivity

Fig. (3) shows the relation between $\ln\sigma_{ac}(\omega)$ and $\ln\omega$ for bulk $CdSe_xTe_{1-x}$ ($0 \le x \le .4$) at room temperature . It is clear from the figure that $\sigma_{ac}(\omega)$ increases with increasing frequency according to equation (2)[20].

$$\sigma_{ac}(\omega) = \sigma_{tot}(\omega) - \sigma_{dc} = B\,\omega^s \qquad (2)$$

where ω is the angular frequency, $\sigma_{tot}(\omega)$ is the measured total electrical conductivity, σ_{dc} is the dc electrical conductivity, s is the frequency exponent and B is constant dependent on temperature.

It is indicated also that $\sigma_{ac}(\omega)$ at any frequency increases with increasing Se content. This is consistent with the increase of dc electrical conductivity with molar fraction x. Fig.(4) shows the relation between $\ln \sigma_{ac}$ and $\ln\omega$ for $CdSe_{0.1}Te_{0.9}$ at different temperatures as a representative example. It is indicated from the figures that σ_{ac} increases with frequency at the elevated temperatures as well as at room temperature for at higher values of frequency. Values of the frequency exponent s at different temperature values in the investigated range were calculated for all the studied compositions from the slopes of the linear part of the relation of $\ln \sigma_{ac}(\omega) = f(\omega)$. The temperature dependence of s

for the investigated compositions is shown in Fig. (5). It is clear from the figure that s decreases as the temperature increases for all compositions.

According to correlated barrier hopping (CBH) model[17-19], the frequency exponent s is ranged from 0.7 to 1 at room temperature, and is found to decrease with increasing temperature, as

$$s = 1 - \frac{6kT}{W_M + [kT \ln(\omega\tau_o)]} \qquad (3)$$

The obtained data for s satisfies this equation, so the frequency dependence of $\sigma_{ac}(\omega)$ can be explained satisfactorily in terms of the CBH model.

The temperature dependence of the ac conductivity $\sigma_{ac}(\omega)$ at different frequencies was studied for $CdSe_xTe_{1-x}$ ($0 \leq x \leq .4$). Fig. (6) shows the plot of ln $\sigma_{ac}(\omega)$ against 1000/T for $CdSe_{0.1}Te_{0.9}$ as a representative example. It is clear from the figure that $\ln\sigma_{ac}(\omega)$ increases nonlinearly with absolute temperature. The same results are obtained for other compositions. If $\ln\sigma_{ac}(\omega)$ depends linearly on the temperature with single activation energy, the mechanism is due to hopping between states near the mobility edges where the density of states is taken to be constant [21] but the obtained dependence is not linear. A possible explanation of this behavior may be that the density of states rises continuously toward the band edges.

3.3 Frequency and temperature dependences of dielectric constant ε_1

Frequency and temperature dependence of dielectric constant ε_1 were studied for the investigated compositions in the investigated ranges of frequency and temperature. The frequency dependence of the dielectric

constant ε_1 at room temperature is shown in Fig.(7). It is clear that ε_1 decreases with increasing frequency. The decrease of ε_1 with frequency can be attributed to the fact that at low frequencies ε_1 for polar materials is due to the contribution of multi component of polarization, deformational polarization (electronic and ionic) and relaxation polarization (orientation and interfacial). When the frequency is increased the dipoles can not rotate sufficiently rapidly, so that their oscillations lag behind those of the field. As the frequency is further increased dipoles will be completely unable to follow the field and the orientation polarization stopped, so ε_1 decreases approaching a constant value at high frequencies due to the interfacial polarization only.

It is indicated also that ε_1 at any frequency increases with the increase of Se content. The same results are obtained at elevated temperatures, as well as, at room temperature for all investigated compositions as indicated in Fig.(8) for $CdSe_{0.4}Te_{0.6}$ as a representative example.

Fig. (9) shows the temperature dependence of the dielectric constant ε_1 at different frequency values for $CdSe_{0.4}Te_{0.6}$ as a representative examples. It is clear that ε_1 increases as the temperature increases. The same results are obtained for all investigated compositions. The increase of ε_1 with temperature can be attributed to the fact that dipoles in polar materials can not orient themselves at low temperatures. When the temperature is increased the orientation of dipoles is facilitated and this increases the orientational polarization, and in turn increases ε_1.

3.4 Frequency and temperature dependencies of the dielectric loss ε_2

Frequency dependence of the dielectric loss ε_2 are studied for the investigated compositions in the considered frequency and temperature

ranges. As a representative example, the relation between ε_2 and lnω is represented in figure (10) for CdTe. It is clear from this figure that ε_2 decreases with increasing frequency in the investigated temperature range. The same results are obtained for all compositions under test. The decrease of ε_2 with frequency can be attributed to the fact that at low frequencies, the value of ε_2 is due to the migration of ions in the material. At moderate frequencies ε_2 is due to the contribution of ions jump, conduction loss of ions migration, and ions polarization loss. At high frequencies ion vibrations may be the only source of dielectric **loss**.

The Frequency dependence of the dielectric loss ε_2 measured at room temperature for investigated compositions is shown in figure (11). It is clear from the figure that ε_2 increases with increasing x. This is consistent with the increase of ac conductivity with x, since ac conductivity is related to ε_2 by the following relation:

$$\sigma_{ac}(\omega) = \varepsilon_o \omega \varepsilon_2(\omega) \qquad (4)$$

Fig.(12) shows the temperature dependence of the dielectric loss ε_2 for CdTe as a representative example. It is clear that ε_2 increases with increasing temperature. The same results are obtained for all compositions under test. Since the dielectric relaxation studies are important to understand the origin of dielectric losses in a material, the variation of ε_2 with temperature can be explained as Steveles[22] who divided the relaxation phenomena into three parts: conduction losses, dipole losses, and vibrational losses. At low temperatures, conduction losses have minimum value since it is proportional to (σ/ω). As the temperature increases σ increases and so the conduction losses increases. This increases the value of ε_2 with increasing temperature.

References

1- G. Hodes, Nature (B)., 285(1980)29.

2- T. H. Weng, J. Electrochem. Soc., 117(1970)725.

3- M. I. Izakron, N. Ya. Karasik, L. M. Prokator, D. A. Sakreev, G. A. Federova, I. N. Yakimenko, Inorg. Mater., 15(1979)178.

4- A. I. Strauss and I. Steinger, J. Electrochem. Soc., 117(1970)1420.

5- Jae-Hyeong Lee, Dong-Gun Lim and Jun-Sin Yi Solar Energy Materials & Solar Cells.,75(2003)235.

6- M. Shamsuddin, A.Nasar, and V. B. Tare, J. Appl. Phys., 74(1993)6208.

7- A. P. Belyaev and I. P. Kalinkin, Thin Solid Films., 158(1988)25.

8-A.P.Belyaev and I.P. Kalinkin, Sov. Phys. Semicond., 20(1986)1078.

9- S. Uthanna and P. Jayarama Reddy, Solid State Comm., 45(1983)979.

10- A.P.Belyaev ,I.P. Kalinkin and V. A. Sanitarov, Sov. Phys. Semicond., 18(1984)1234.

11- A.P.Belyaev, I.P. Kalinkin and V. A. Sanitarov, Sov. Phys. Semicond., 19(1985)95.

12- L. D. Budyonnaya, A. M. Parelets, L. N. Khanat and V. E. Badan, Thin Solid Films., 138(1986)163.

13- M. M. El-Nahass, M. M. Sallam, M. A. Afifi, I. T. Zedan, Materials Research Bulletin., 42(2007)371.

14- M.Pollak, Phil. Mag., 23(1971) 519.

15- M.Pollak, T.H.Geballe, Phys Rev B., 22(1961)1742.

16- A.R.Long , Adv. Phys., 31(1982)553.

17- S.R.Elliott, Phil. Mag. B., 36(1978)1291.

18- S.R.Elliott, Phil. Mag. B., 37(1978)135.

19- K.Shimakawa , Phil. Mag., 46(1982)123.

20- A.K.Jonscher, Nature., 267(1977)673.

21- H. K. Rockstad, J. Non-Crystal. Solid., 8(1972)621.

22- J.M.Stevels, "The Electrical Properties of Glasses", Hand buch der Physik., (1975)350.

Table (1)

Dc activation energy (ΔE) and optical energy gap (E_g^{opt})for $CdSe_xTe_{1-x}$

composition	ΔE, eV	E_g^{opt}, eV
CdTe	0.596	2.556
$CdTe_{0.9}Se_{0.1}$	0.391	2.507
$CdTe_{0.8}Se_{0.2}$	0.267	2.46
$CdTe_{0.7}Se_{0.3}$	0.254	2.43
$CdTe_{0.6}Se_{0.4}$	0.238	2.4

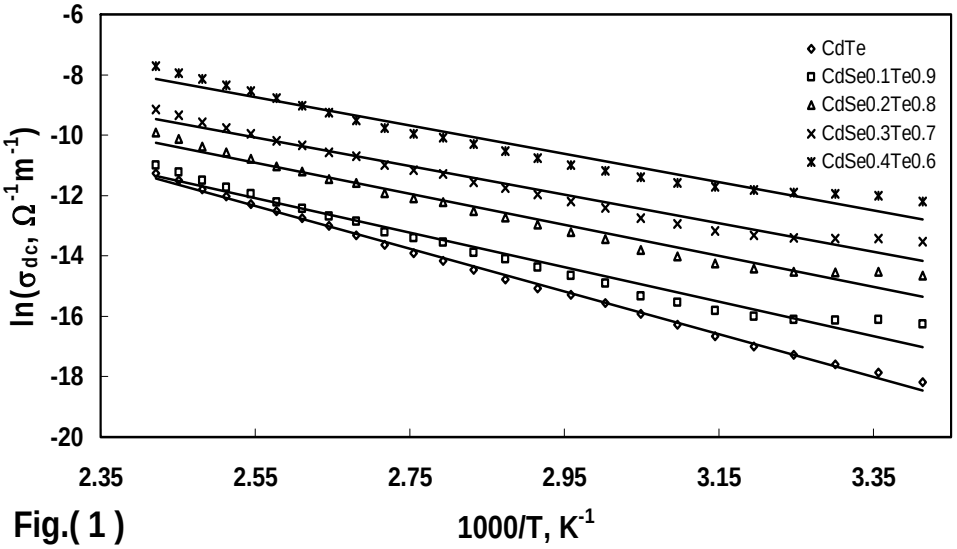

Fig.(1)

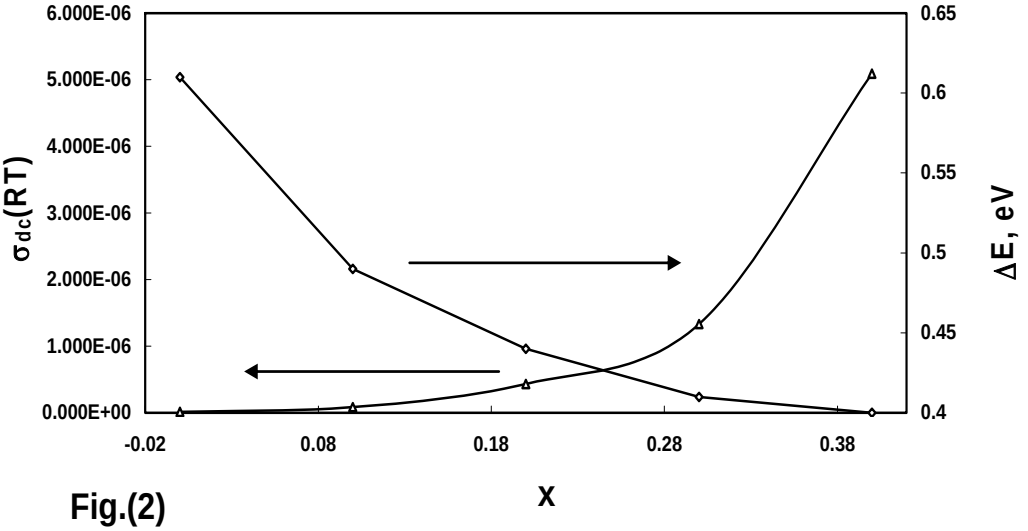
6.000E-06
5.000E-06
4.000E-06
3.000E-06
2.000E-06
1.000E-06
0.000E+00
σdc(RT)
0.65
0.6
0.55
0.5
0.45
0.4
ΔE, eV
-0.02
0.08
0.18
0.28
0.38
X

Fig.(2)

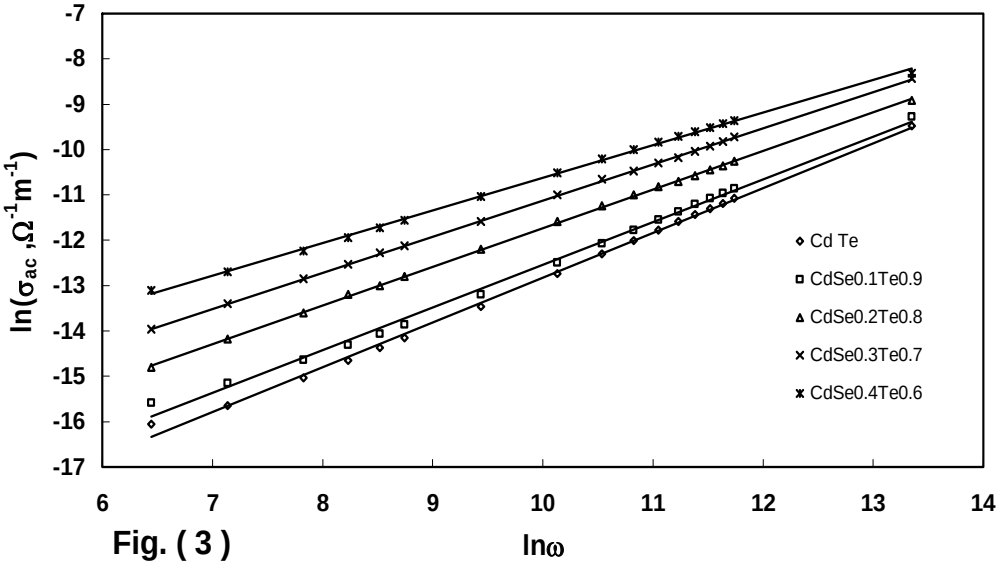
-7
-8
-9
-10
-11
-12
-13
-14
-15
-16
-17
6
7
8
9
10
11
12
13
14
ln(σac ,Ω-1m-1)
lnω
Cd Te
CdSe0.1Te0.9
CdSe0.2Te0.8
CdSe0.3Te0.7
CdSe0.4Te0.6

Fig. (3)

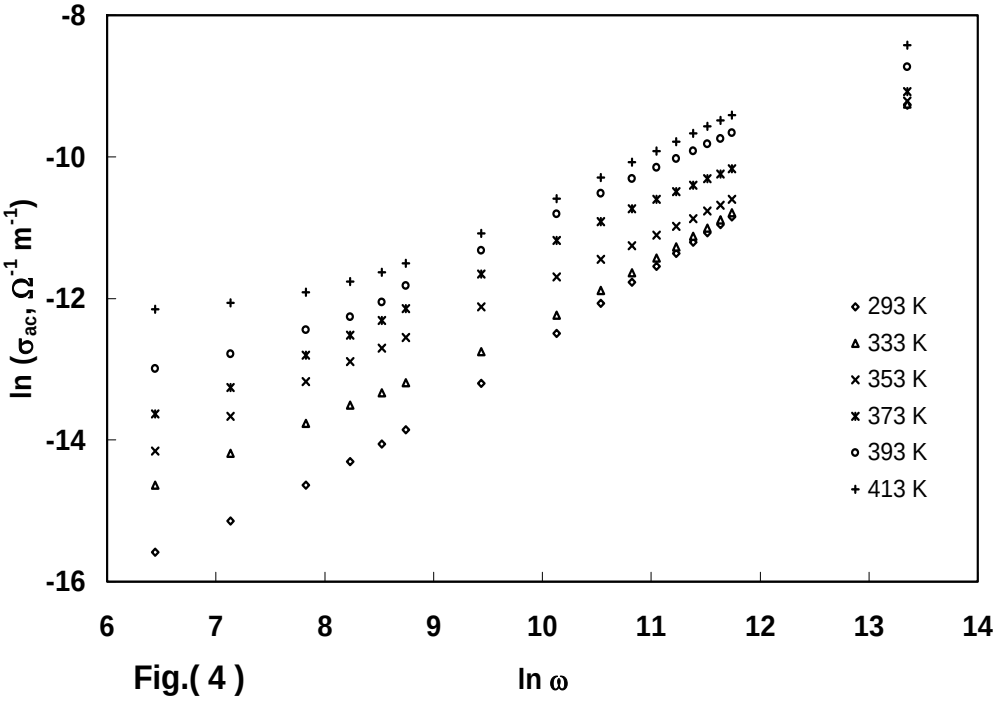
-8
-10
-12
-14
-16
6
7
8
9
10
11
12
13
14
ln (σac, Ω-1 m-1)
ln ω
293 K
333 K
353 K
373 K
393 K
413 K

Fig.(4)

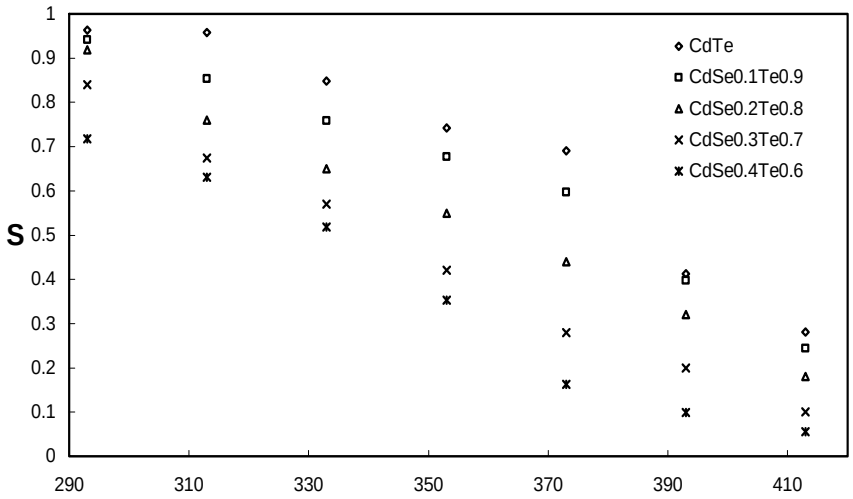
S
T, K
CdTe
CdSe0.1Te0.9
CdSe0.2Te0.8
CdSe0.3Te0.7
CdSe0.4Te0.6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
290
310
330
350
370
390
410

Fig.(5)