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On the study of electrical conductivity of polycrystalline cadmium telluride

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The complex impedance of polycrystalline cadmium telluride has been measured as a function of frequency by a two-probe technique. The experimental data measured in the temperature range 301–565 K have been analyzed in the complex plane formalism and suitable equivalent circuits have been proposed in different temperature regions. The values of resistance and capacitance of bulk and grain boundary contributions have also been independently calculated from the Debye peak of spectroscopic plots. The role of bulk and grain boundary in the overall conduction process have been discussed with realistic justification.

1. Introduction

Cadmium telluride (CdTe), belongs to the family of direct band gap semiconductors. The compound is an important material in semiconductor technology due to increasing applications in various electronic devices [1, 2] such as room temperature X-ray and γ-ray detectors, electro-optical and acousto-optical modulators, partial reflector, high efficient solar cells etc. Although there has been greater emphasis on the characterization and development of single crystal of CdTe as electronic material the polycrystalline compound has received considerable attention in recent years because of ease and negligible cost of synthesis.

A literature survey reveals that studies on the polycrystalline CdTe are concerned with the electrical characterization based on the d.c. measurements and so far no attempt has been made to study this compound by measuring the a.c. conductivity although the latter gives important information about various factors contributing to the overall conduction mechanism. Since in polycrystalline materials the grain boundary play a considerable role in the conduction process it is worth separating the conductivity due to grain boundary from that of bulk.

The electrical conductivity of polycrystalline materials has been thoroughly discussed in terms of bulk and grain boundary effects by a number of investigators [e.g., 3–8]. Recently some work on the compound semiconuctors such as PbTe [9] and ZnS [10] based on a.c. conductivity measurements have been reported. In the present work the complex impedance of polycrystalline CdTe has been measured over a wide range of frequencies (10 Hz–10 MHz) at different temperatures with the prime objective to analyze whether the overall conduction is dominated by the bulk or the grain boundary and also to assess the quality of the electrical homogeneity of the sample.

2. Theory

Impedance analysis provides a simple method to determine various contributions of the total conductivity of electrical materials in terms of four possible complex formalisms, viz., impedance (Z^*), admittance (Y^*), modulus (M^*) and permittivity (E^*). These parameters are interrelated as [3]:

$$Z^* = (Y^*)^{-1} \tag{1}$$

$$Y^* = j\omega C_0 E^* \tag{2}$$

$$E^* = (M^*)^{-1} \tag{3}$$

$$M^* = j\omega C_0 Z^* \tag{4}$$

where, ω is angular frequency and C_0 is the vacuum capacitance of the measuring cell and electrodes having air gap in place of sample and defined as

$$C_0 = e_0(a/l) \tag{5}$$

where e_0 is the permittivity of the free space (8.854×10^{-14} F/cm), and a and l are the cross sectional area and thickness of cylindrical sample.

Impedance is a more general and useful quantity than resistance because it takes both resistive (real) and reactive (imaginary) components into account:

$$Z^* = Z' - jZ'' \tag{6}$$

The complex impedance plane analysis is based on the plot of imaginary part (Z'') against real part (Z') of the total impedance over a wide range of frequencies. The plot gives single or a series of semicircular arcs. Each semicircular arc represents the parallel combination of resistance (R) and capacitance (C) of the respective species taking part in the conduction process. The arc in highest frequency range, passes through the origin, represents bulk contribution. In the intermediate frequency range, the arc represents the grain boundary contribution where as in the lowest frequency range it highlights the role of sample-electrode interface or electrode polarization.

From the intercept of arc with real axis, values of R and C are calculated. Best results are obtained by using a combination of impedance and modulus plane analyses along with the spectroscopic plots of imaginary components (Z'' and M'') against logarithm of frequency.

3. Experimental

High purity (99.999% pure) cadmium and tellurium elements, obtained from Johnson Matthey (U.K.) were used in the present investigation. The stoichiometric mixture of cadmium and tellurium corresponding to the composition CdTe, weighed to an accuracy of 10^{-5} gm, was sealed in a silica capsule under a vacuum of 1.3×10^{-8} atm. The capsule was first heated at a rate of about 3 K/min to a temperature of 1415 K, 50 K above the melting point of CdTe, then held for about 24 hours with periodic shaking and finally quenched in cold water. The resultant mass was crushed into fine powder and then compressed (at the pressure of 70 Kg/cm^2) to form cylindrical pellet (diameter: 0.708 cm and thickness: 0.394 cm) by means of die and punch. The pellet was sintered at 950 K for about 72 hours in a sealed silica capsule under the vacuum of the same order. The flat surfaces of the sintered pellet were polished and then coated with a thin layer of high temperature silver paint (Eltecks Corpn., India).

A two-probe sample holder cell assembly schematically shown in Fig. 1, was made of two piston type silica tubes. The sintered and polished CdTe pellet placed between two silver discs was pressed by two open end silica tubes with the aid of nichrome springs. To each of the silver discs one silver wire was welded. The silver electrode wires were taken out from the slotted portion of the outer silica tube. The sample holder assembly was placed in one end closed silica tube by the support of argon inlet silica tube. The entire experimental assembly, kept in a horizental furnace, was evacuated to 1.3×10^{-5} atm and purged with high purity argon repeatedly three/four times.

The impedance (Z^*) of CdTe was measured as a function of frequency (10 Hz–10 MHz) in the temperature range of 301–565 K by Impedance Analyzer (Hewlett Packard, Japan; Model: 4192 A LF). In order to check the reproducibility of the results, measurements were conducted during heating as well as cooling cycles.

4. Results and discussion

The variation of imaginary part with the real part of the total complex impedance measured over a wide range of frequencies is shown in Fig. 2 at three typical temperatures, viz., 301, 375 and 456 K. From Fig. 2a it is clear that in the high frequency region there is one semicircular arc passing through the origin. This arc is due to the parallel combination of bulk resistance (R_1) and bulk capacitance (C_1) of CdTe. The second arc has not been resolved. This indicates that the resistance of grain boundary is very high in comparison to the bulk. Thus the conductivity of sample is dominated by grains and role of grain boundary is negligible in conduction process at 301 K.

As the temperature of sample increases to 349 K another semicircular arc appears in the low frequency region. Two semicircular arcs in the impedance plots have been observed in an intermediate temperature range of 349–401 K. The impedance plots showing two arcs in different frequency regions is shown in Fig. 2b at 375 K. The first arc in the high frequency region passing through the origin is due to the parallel combination of bulk resistance (R_1) and bulk capacitance (C_1) and the second arc in the low frequency region is due to the parallel combination of grain boundary resistance (R_2) and grain boundary capacitance (C_2). From Fig. 2b it is evident that R_2 is about 30 times larger than R_1. Thus the conductivity of CdTe at this temperature is still dominated by grains though the role of grain boundary in the conduction process cannot be ignored. In this context it is important to mention that in this intermediate temperature range (349–401 K) the role of grain boundary in conduction process increases with increase of temperature.

It is interesting to note that size of high frequency arc corresponding to bulk effect decreases with increase of temperature and disappeared at 426 K and only one arc shifted from origin is obtained in the high temperature region of 426–565 K. One such plot is shown in

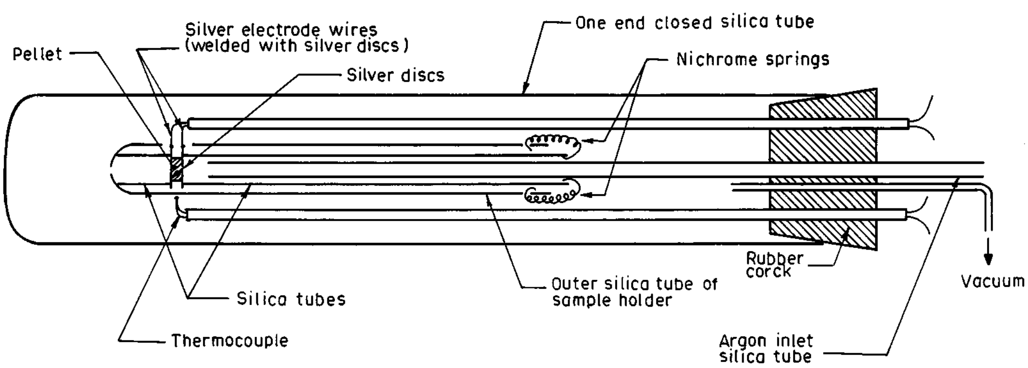

Figure 1 Schematic diagram of experimental cell assembly.

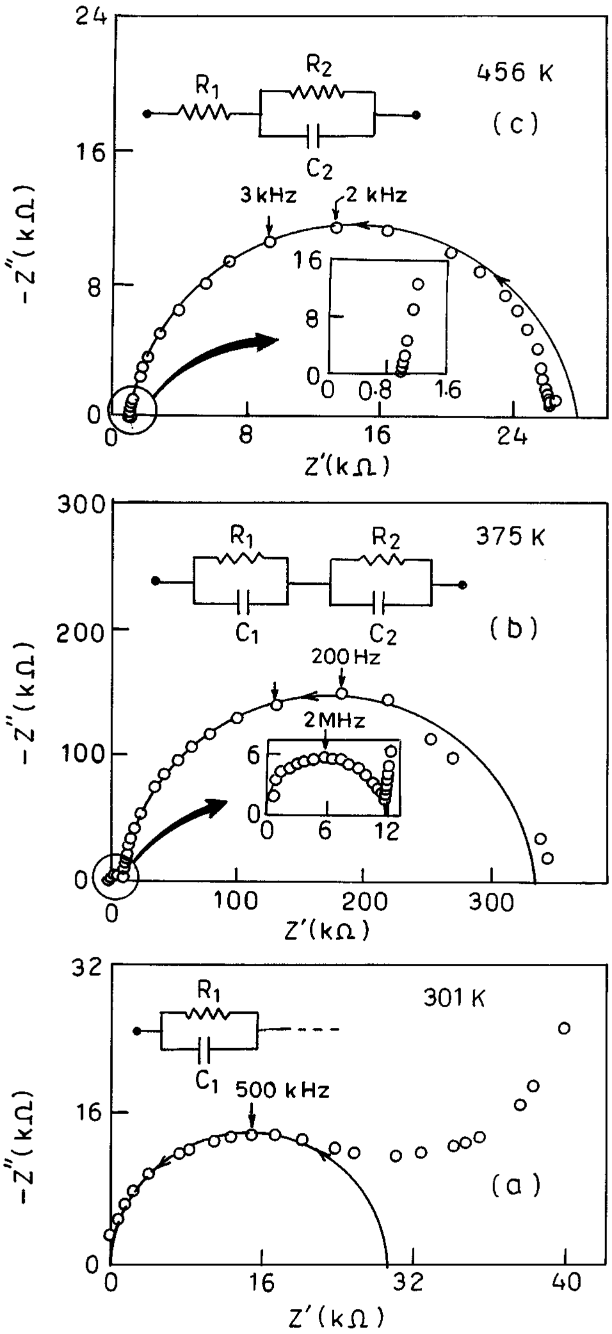

Figure 2 Complex impedance plots at different temperatures.

Fig. 2c at 456 K. The arc intercepts the real axis at R_1 and $R_1 + R_2$ (where R_1 and R_2 are the bulk and grain boundary resistances, respectively). This figure also indicates that the conductivity of polycrystalline CdTe is again mainly due to grains.

From Fig. 2 it is clear that the centre of each arc either lies on the real axis or very close to the real axis i.e. angle of depression is negligible. This clearly highlights that our polycrystalline sample is electrically homogeneous and associated with single relaxation time.

From the values of bulk and grain boundary resistances, respective values of capacitance have been calculated by using the following relationship:

$$2\pi f_{\max} RC = 1 \qquad (7)$$

where, $f_{\max}$ is frequency of peak maxima. Since in the complex impedance plane analysis the response is dominated by the arc with larger resistance where as in the modulus plane the response is dominated by the arc with smaller capacitance, a compromise has been made while selecting the values of resistance and capacitance. However, it has been observed that different values of R and C as obtained by complex impedance and modulus analyses are in very good agreement. The values of bulk capacitance ($C_1 = 7.7$ pF) and grain boundary capacitance ($C_2 = 2.1$ nF) so selected have been found to be independent of temperature. The temperature independent values of the capacitance are consistent with the non-ferroelectric nature of CdTe.

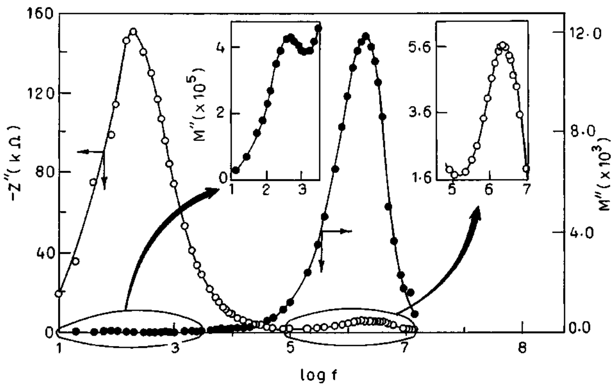

Figure 3 Impedance and modulus spectroscopic plots at different temperatures.

Different values of resistance and capacitance have also been independently calculated from the Debye peak of the spectroscopic plot. In this method the imaginary parts of complex impedance and modulus are plotted against logarithm of frequency and the peak height in Z'' and M'' plots give respective values of $R/2$ and $C_0/2C$. The values of Z'' and M'' are plotted against $\log f$ in Fig. 3 at 375 K in the intermediate temperature range where both the peaks of bulk and grain boundary effects are expected. From Fig. 3 it is evident that Z'' plot gives a large peak in low frequency region corresponding to the grain boundary effect where as M'' gives dominating peak in the high frequency region corresponding to the bulk effect. As the values of bulk resistance is much lower than that of the grain boundary and similarly the value of grain boundary capacitance is much higher than the bulk capacitance; their corresponding peaks could not be resolved in the normal scale. In order to obtain bulk resistance and grain boundary capacitance the corresponding plots in limited frequency range have been amplified and shown in boxes in Fig. 3. The values of resistance and capacitance as obtained from the spectroscopic plot have been found to be in excellent agreement with those calculated from the traditional complex impedance and modulus plane analyses.

Fig. 4 shows the modulus spectroscopic plots at different temperatures in the frequency region of bulk contribution. From the figure it is clear that position of peak moves to higher frequency side with the increase of temperature except at 349 K. Further the peak height remains constant except at 301 K. This also indicates the temperature independent nature of capacitance.

The values of resistance of bulk and grain boundary contributions at different temperatures have been used

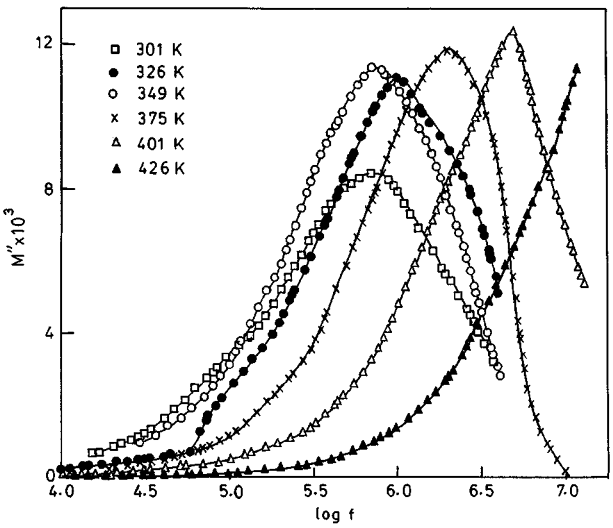

Figure 4 Modulus spectroscopic plots at different temperatures.

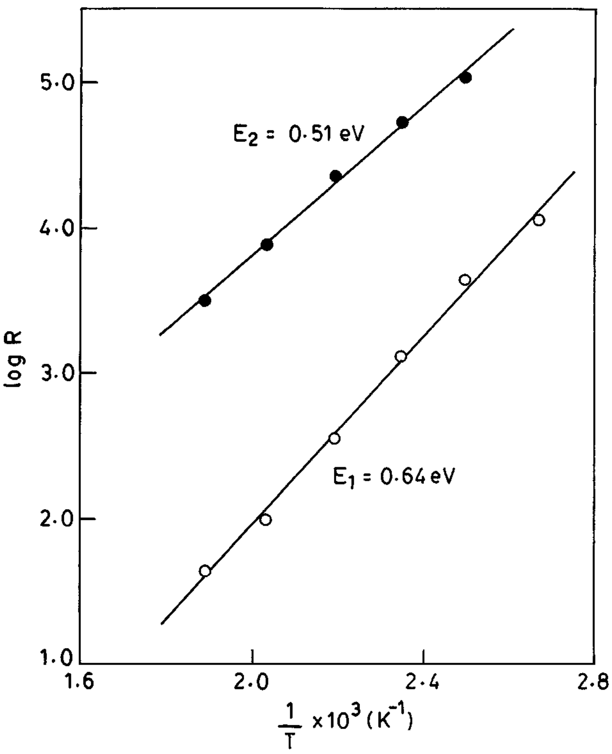

Figure 5 Arrhenius plots for R_1 and R_2.

to finally calculate the activation energy of the conduction process. The variation of logarithm of bulk and grain boundary resistances have been plotted against inverse of temperature in Fig. 5. The plot shows two different lines for bulk and grain boundary effects. The corresponding values of activation energies for bulk conduction (0.64 eV) is slightly higher than grain boundary conduction process (0.51 eV). The band gap of CdTe has been reported to be 1.58 eV [2]. The lower value of activation energy for bulk conduction obtained in the present investigation is likely to be due to the presence of impurity during preparation of the sample or due to diffusion of silver atoms from the surface coating.

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