

Structural, optical, photoluminescence, dielectric and electrical studies of vacuum-evaporated CdTe thin films

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Abstract. Highly-oriented CdTe thin films were fabricated on quartz and glass substrates by thermal evaporation technique in the vacuum of about 2×10^{-5} torr. The CdTe thin films were characterized by X-ray diffraction (XRD), UV–VIS–NIR, photoluminescence spectroscopy and scanning electron microscopy (SEM). X-ray diffraction results showed that the films were polycrystalline with cubic structure and had preferred growth of grains along the (111) crystallographic direction. Scanning electron micrographs showed that the growth of crystallites of comparable size on both the substrates. At the room temperature, photoluminescence spectra of the films on both the substrates showed sharp peaks with a maximum at 805 nm. This band showed significant narrowing suggesting that it originates from the transitions involving grain boundary defects. The refractive index of CdTe thin films was calculated using interference pattern of transmission spectra. The optical band gap of thin films was found to allow direct transition with energy gap of 1.47–1.50 eV. a.c. conductivity of CdTe thin films was found to increase with the increase in frequency whereas dielectric constant was observed to decrease with the increase in frequency.

Keywords. CdTe; optical properties; photoluminescence; SEM; a.c. conductivity.

1. Introduction

Cadmium telluride (CdTe) is an important group II–VI semiconductor with a direct band gap of 1.5 eV at room temperature. Extensive research was done in the last two decades on CdTe thin films, mainly due to its potential applications, particularly in the field of polycrystalline thin film solar cells and also large area electronic devices like field-effect transistors, radiation detector, optical thin film filters, nonlinear integrated optical devices, light emitting diodes (LEDs) and laser heterostructures for emission in the infrared spectral range (Goldsmid *et al* 1980; Patel and Patel 1992; Nair *et al* 1993; Cruz *et al* 1999; Romeo *et al* 2001; Van Gheluwe *et al* 2005). The absorption edge in CdTe is very sharp due to its direct energy band gap and thus efficiency of absorption of light is very high around 90%. The maximum theoretical efficiency reported for CdTe solar cells is 29%. Whereas the conversion efficiency of CdTe solar cell was reported up to 16.5% (Kosyachenko *et al* 2009). Still, the conversion efficiency, crystallites size, optical properties and conduction phenomena in CdTe thin films are some open-ended problems demanding extensive research. The growth of high-quality and low-cost CdTe polycrystalline thin films for producing high conversion efficiency solar cells is the current topic of research. CdTe/CdS solar cells are one of the prospective candidates for widespread commercial

success in solar energy conversion and also for use as a substrate for the important infrared detector material HgCdTe, dilute magnetic semiconductor, epitaxial layers and quantum well structures (Morales-Acevedo 2006; Robin *et al* 2009).

A number of techniques of deposition were adopted to obtain CdTe thin films (Feldman *et al* 1981; Gongoi and Barua 1982; Anthony *et al* 1984; Matsumoto *et al* 1984; Takahashi *et al* 1984; Wang and Reinhard 1984; Matsumura *et al* 1985; Gayle and Biancaniello 1995). All these techniques have their own merits and demerits in producing high-quality CdTe films. Among various other techniques, thermal evaporation techniques are simple and economical. Recently structural and optical properties of thermally-evaporated CdTe polycrystalline thin films were reported (Lalitha *et al* 2007; Al-Ghamdi *et al* 2010), however the work on important parameters like nucleation of grain size, microstructures and how to affect various properties of polycrystalline CdTe thin films is still to be done (Bacaksiz *et al* 2007; Semaltianos *et al* 2009). In the present work, the microstructural, optical, dielectric and electrical, and photoluminescence properties of CdTe thin films fabricated on glass and quartz substrates were investigated.

2. Experimental

Analytical grade CdTe powder with 99.99% purity was purchased from Alfa Aesar (UK). CdTe thin films were fabricated by thermal evaporation technique in a vacuum about 2×10^{-5} torr, using vacuum coating unit. Molybdenum boat

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was used as the evaporation source and quartz and glass substrates were placed directly above the source at a distance of nearly 15 cm. The quartz and glass substrates were cleaned with freshly prepared acetone, detergent solution and distilled water, respectively. Further, the substrates were subjected to ultrasonic cleaning prior to the evaporation of CdTe. The transmittance spectra for as-deposited CdTe thin films on glass and quartz substrates were obtained in the range of 190–2500 nm using JASCO UV–VIS–NIR spectrometers (Model-V570). The structure of the films was studied using Philips analytical diffractometer (Model PW3710). The Photo luminescence (PL) measurement at an excitation wavelength of 525 nm was carried out using an Ar-ion laser with the maximum output power of 200 mW. The surface morphology of CdTe thin films was performed by the JSM-6700 scanning electron microscope. The dielectric properties like dielectric constant (ϵ_r) and loss tangent ($\tan \delta$) of the films were calculated from the a.c. measurements of impedance, capacitance and phase angle measured as a function of frequency using agilent impedance analyser (model-4294A).

3. Results and discussion

3.1 X-ray diffraction analysis

XRD patterns of CdTe thin films on different substrates are shown in figure 1, whereas the XRD pattern of CdTe powder are presented in figure 2. XRD analysis of the thin films indicated the cubic structure with peaks at $2\theta = 23.51^\circ$, 39.20° and 46.18° with the orientations (1 1 1), (2 2 0) and (3 1 1), respectively. It was observed that the CdTe crystallites have similar growth on quartz and glass substrates along (1 1 1) index. For the calculation of grain size and strain of CdTe thin films on glass and quartz substrates, we have used Williamson method, which was first proposed by Williamson and Hall and is customarily referred as Williamson Hall method. The equation for the separation of crystallites size and the strain takes the following form (Semaltianos *et al* 1995):

$$\beta \cos \theta = \lambda/D_v + 4\varepsilon (\sin \theta), \quad (1)$$

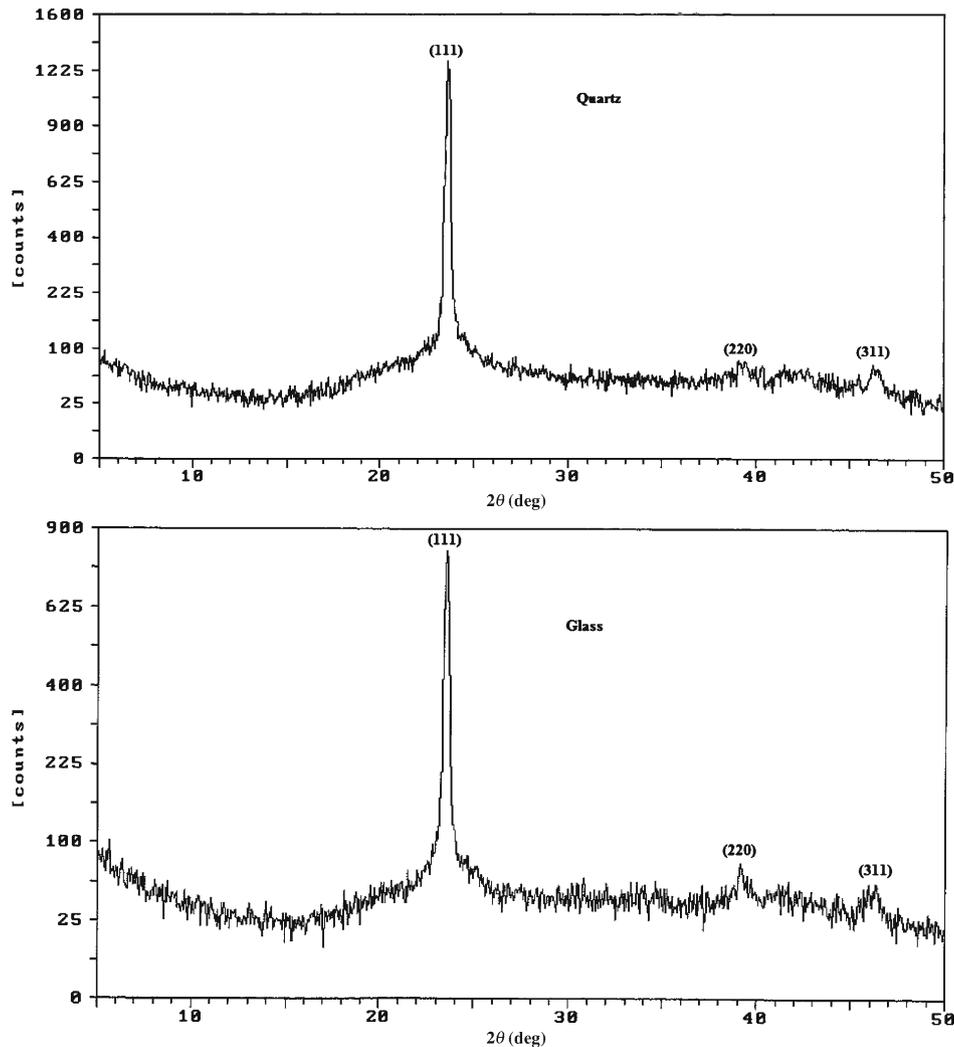


Figure 1. XRD patterns of CdTe thin films on glass and quartz substrates.

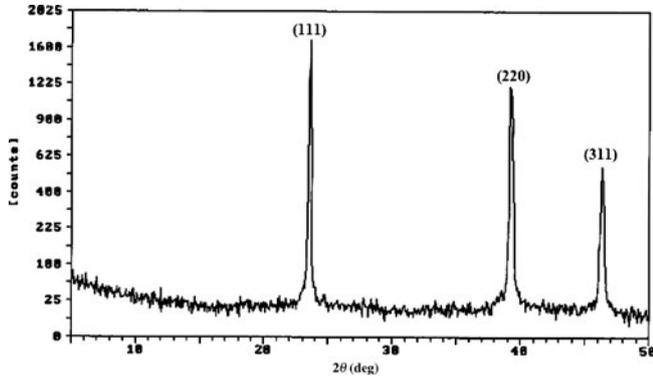


Figure 2. XRD pattern of CdTe powder.

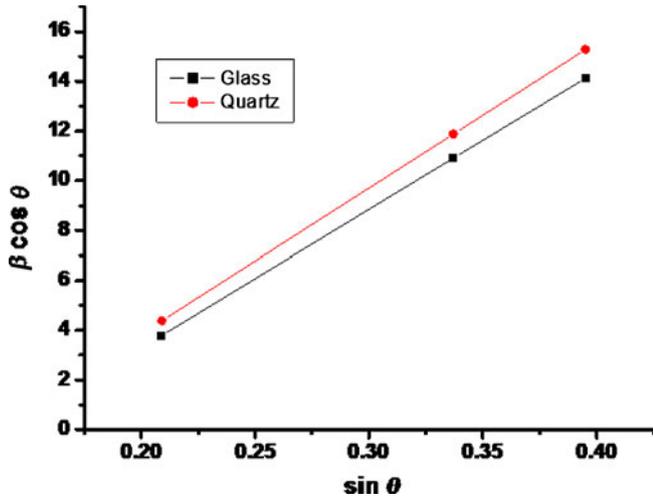


Figure 3. Grain size and strain calculated using Williamson-Hall method.

where λ is the wavelength of X-ray used (1.54 \AA in our case) and D_v , ε are the grain size and strain, respectively.

The peak width at half maximum β of each reflection to be used in (1) is calculated using relation (Shaaban *et al* 2009):

$$\beta = B (1 - b^2/B^2) \text{ (rad.)}, \quad (2)$$

where B and b are the width of the same Bragg-peak from the XRD pattern of thin film and CdTe powder, respectively. The plots $\beta \cos \theta$ vs $\sin \theta$ for the film on glass and quartz substrates are shown in figure 3. The values of grain size and strain are calculated from ordinate-intersection and slope of the graph, respectively. The values of width, grain size and strain of each reflection of CdTe thin films on different substrates are given in table 1, from which it was observed that the strain is slightly more in films on quartz substrates than on the glass substrates.

3.2 Optical properties

Optical properties of CdTe thin films on glass and quartz substrates are discussed in this section. Transmission spectra

Table 1. Comparative view of breadth, grain size and strain of CdTe thin films on glass and quartz.

Substrates	β			Grain size (nm)	Strain	Band-gap (eV)
	(111)	(220)	(311)			
Glass	0.00209	0.01158	0.01669	45	0.0138	1.50
Quartz	0.00448	0.01266	0.01664	56	0.0143	1.47

of CdTe thin films are shown in figure 4. The transmission of the thin films in the spectral range of 1000–2500 nm is found to be very high. This confirms that the thin films have semiconducting properties; as it is an established fact that the pure semiconducting compounds have a sharp absorption edge (Nowak 1995). The well-known relation near the fundamental absorption edge is given by

$$\alpha = A (h\nu - E_g)_{h\nu}^m, \quad (3)$$

where A is the characteristic parameter (independent of photon energy) for this transition, h the Plank's constant, ν the frequency of light, E_g the band gap and m the parameter which characterizes the transition process involved. The parameter m takes the values of 2 and 1/2 for the direct allowed transition and for indirect allowed transition, respectively. In the case of CdTe polycrystalline thin films on different substrates the direct transitions are valid. The plots $(\alpha h\nu)^2$ vs $h\nu$ for the polycrystalline CdTe thin films on glass and quartz substrates are shown in figure 5. The values of energy band gap of the thin films as determined by extrapolation of linear portion of the plots $(\alpha h\nu)^2$ against $h\nu$ to the energy axis. The calculated band gap for both the films is found to be in the range of 1.47–1.50 eV, which is in good agreement with its reported values for the CdTe thin films (Khairnar *et al* 2003). The energy band gap value of CdTe thin films on glass substrates is found to be more than that of the film deposited on quartz substrate.

The refractive index is determined using the method of recording envelopes around the interference maxima and minima in the transmittance spectra (Swanepoel 1983). Following Swanepoel method, the value of refractive index at a particular wavelength can be calculated using the expression:

$$n = \left[N + (N - S^2)^{1/2} \right]^{1/2}, \quad (4)$$

where

$$N = 2S \frac{T_{\max} - T_{\min}}{T_{\max} T_{\min}} + \frac{S^2 + 1}{2},$$

where T_{\max} and T_{\min} , are the transmittance maximum and the corresponding minimum at a certain wavelength λ . On the other hand, the necessary values of the refractive index of the substrate are obtained from the transmittance spectrum of the

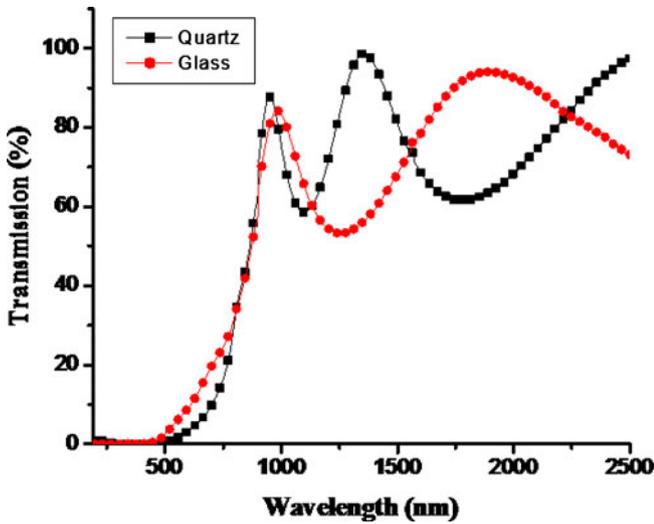


Figure 4. Transmission spectra of CdTe thin films on glass and quartz.

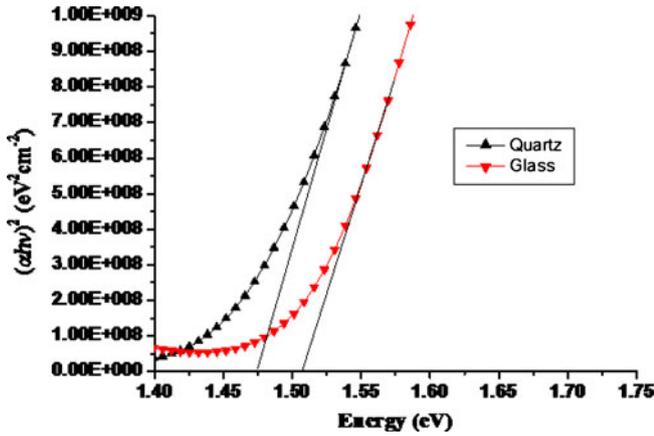


Figure 5. $(\alpha hv)^2$ vs $h\nu$ plots.

substrate, T_s using the well known equation (Rakhshani and Al-Azab 2000):

$$S = \frac{1}{T_s} + \left(\frac{1}{T_s} - 1 \right)^{1/2}. \quad (5)$$

The values of the refractive index, n for CdTe polycrystalline thin films as calculated from (4) are plotted against the wavelength in figure 6. It is observed from these graphs of n vs λ that the refractive index, n decreases with the increase in the wavelength, λ .

3.3 Photoluminescence

Photoluminescence spectra of CdTe polycrystalline thin films on glass and quartz are shown in figure 7. The photoluminescence spectroscopy plays a very important role to determine the exact energy levels of nanostructures or poly-

crystalline thin films. In PL spectra of CdTe films, a strong and narrow emission peak at 805 nm is observed when the sample is excited at 532 nm, showing no trap-related emission. The photoluminescence spectra of CdTe thin films on quartz and glass substrates differ in peaks width (FWHM). The luminescence at 805 nm may be attributed to a higher level transition in CdTe crystallites. The significant narrowing of the band may be due to the growth of round grains shaped with the average size of 50–100 nm and it may involve transitions associated with grain-boundary defects as reported by Marafi *et al* (2003). It was reported that this kind of band-edge luminescence arises from the recombination of exciton and/or shallow trapped electron–hole pairs (Armani *et al* 2007). The film grown on quartz substrates has high peak width ~ 60 meV (FWHM) whereas the film grown on glass substrates has low peak width ~ 10 meV. This difference may be due to the microstructure of the thin films.

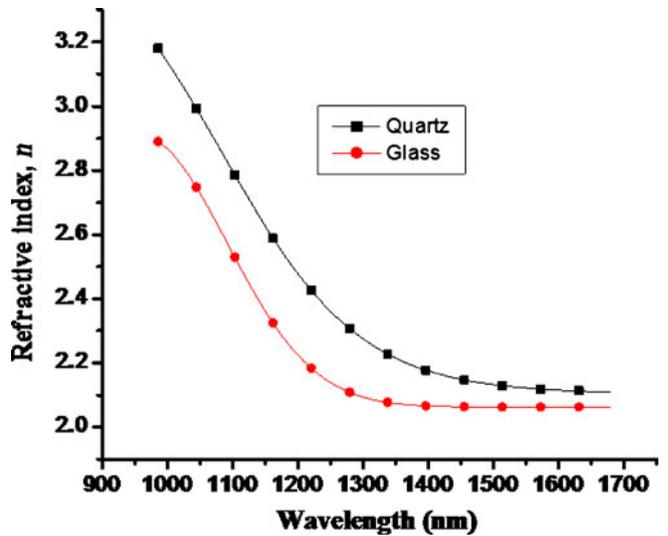


Figure 6. Refractive index of CdTe thin films.

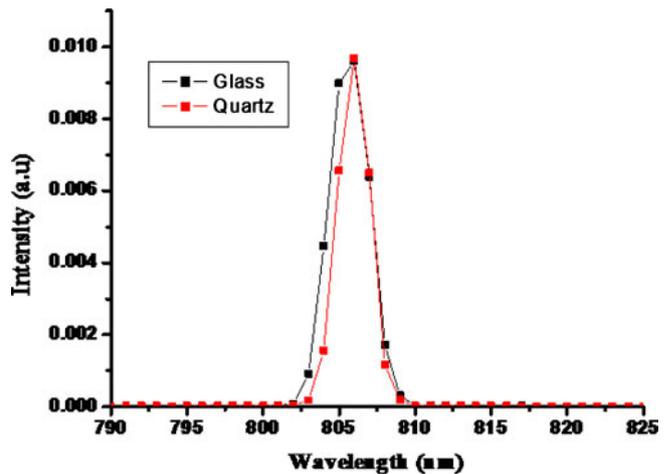


Figure 7. Photoluminescence spectra of CdTe thin films on glass and quartz substrates.

3.4 SEM analysis

Surface morphology of thermally-evaporated CdTe thin films on quartz and glass substrates are shown in figures 8(a), (b). From these SEM micrographs, it is evident that there is small difference in the grain size of films grown on quartz and glass substrates. The substrates are well covered by large round shaped CdTe crystallites of average grain size of 50–100 nm, similar to that obtained using the XRD analysis. Microstructure of CdTe thin films on quartz and glass substrates shows non-uniform growth of grains as was reported by Sharma *et al* (2005).

3.5 Dielectric and electrical properties

The variations of dielectric constant, dielectric loss, $\tan \delta$ and a.c. conductivity with frequency for the CdTe thin films in the frequency range of 10 Hz–100 kHz are shown in figures 9(a)–(c), respectively. The dielectric constant is found to decrease with the increase in frequency. The thin films of CdTe exhibited the similar behaviour in the case of dielectric loss. This type of behaviour suggests a distribution of relaxation times in the CdTe thin films system. The XRD

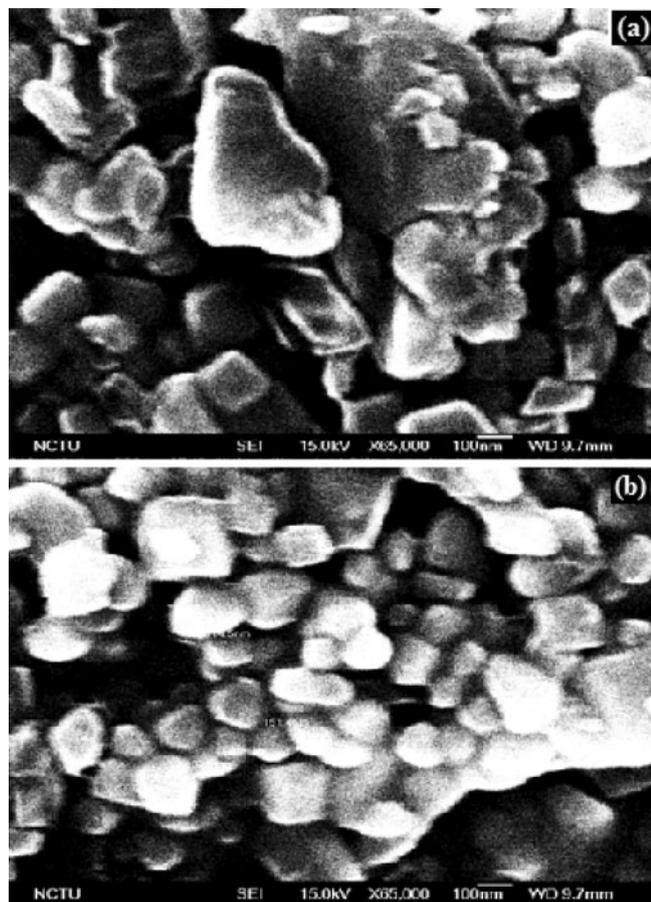


Figure 8. SEM micrograph of CdTe thin films on (a) quartz and (b) glass substrates.

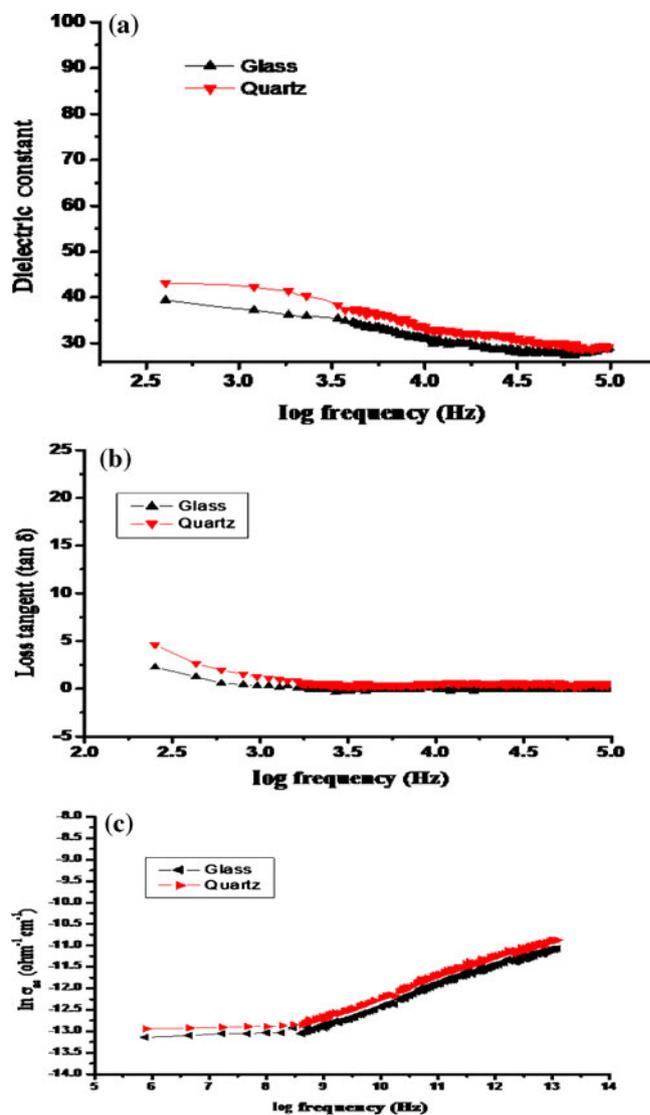


Figure 9. Variations of (a) dielectric constant, (b) loss tangent and (c) a.c. conductivity with frequency.

patterns of thin films have only one intense peak suggesting the noticeable disordered nature of the system, the same is also confirmed from the SEM micrographs. Structural information of thin films suggests simple or multifaceted defects such as defect centres, micro voids, imperfections, cracks, etc that may be present in the films. These defects play very important role in transport phenomena, as these defects originate the defect states like shallow and deep states which may act as donor or acceptors. Such type of states affect the transport phenomena in thin films to a great extent by acting as traps and recombination centres for carriers. These states may also lead to the probable formation of dipoles, which are responsible for the dielectric behaviour. When the thin films are subjected to electric field, the electron hop between localized states. Transport of charge carriers between these sites, hop from a donor to an acceptor state. As a result, each pair of sites forms a dipole and contributes to distributed dielectric relaxation (Prabakar *et al* 2002).

The a.c. conductivity is determined using the relation,

$$\sigma_{ac} = \varepsilon_0 \varepsilon_r \omega \tan \delta. \quad (6)$$

Figure 9(c) displays the variation of a.c. conductivity with frequency. A.c. conductivity of CdTe thin films is found to increase with the frequency. Such type of behaviour is shown commonly by various other materials and was reported in the literature (Mardare and Rusu 2004). The increase in a.c. conductivity with frequency again indicates the existence of localized conduction in CdTe thin films in which the a.c. conductivity increases with increase in frequency. In contrast to this, in the case of free band conduction the a.c. conductivity decreases with increase in frequency (Anwar and Hogarth 1990).

4. Conclusions

The device-grade CdTe polycrystalline thin films were fabricated by the thermal evaporation technique on quartz and glass substrates. The XRD studies have revealed that the thin films are polycrystalline in nature and CdTe crystallites have cubic structure. The structural parameters like grain size and strain were calculated from XRD pattern. Transmission of CdTe thin films is found to be 85–90% in infrared and near infrared region. Energy band gap of thin films is found to be in the range of 1.47–1.50 eV. Refractive index of thin films is very high in infrared region and it is found to decrease gradually with increasing wavelength. SEM studies revealed the columnar growth of CdTe crystallites. Photoluminescence spectra of CdTe thin films showed sharp peaks around 805 nm. Overall investigation suggests that CdTe polycrystalline thin films on quartz and glass substrates have similar properties.

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