Chapter Six

Conclusion and suggestions for further work

6.1. Conclusion

A total of twenty three samples of e-beam sputtered CdTe thin films were characterized in this work. The results of structural, optical and electro-optical studies showed some unique properties which were not previously observed in CdTe films.

Structural characterization by XRD indicates nine of twenty three samples are polycrystalline with preferential orientation in the [111] direction of the zinc-blende structure. The remainder of the samples are of amorphous form. Calculations of the lattice spacing on the polycrystalline samples however revealed a somewhat larger value compared to bulk CdTe which indicates the presence of stress in the films. The magnitude of this expansive stress varied from 1.3×10^9 dyn/cm^2 to 1.7×10^{10} dyn/cm^2. The grain size of the polycrystalline films as determined from XRD varied from 12 to 81nm while observations under SEM and TEM showed larger grain cluster of approximately 1 μm in diameter interspersed between finer grains. In addition variation in grain size with the position of the substrates during deposition was observed.

EDAX analysis of the elemental composition of the films indicated excess Te in all films. This observation is explained by the disassociation of the compound into its constituent atoms of Cd and Te upon evaporation where Te is thought to have a higher sticking coefficient. In the present study an almost linear relation between the density of excess Te with the reciprocal of thickness (see Figure 3.12) seems to lend support to the above hypothesis. The relation of grain size and uniaxial stress with the density of excess Te

were also similarly analyzed (see Figure 3.13 and 3.14). The results indicated with th exception in one or two cases, the former decreased with an increase in the density o excess Te while in the latter an increase is observed with the density of excess Te.

The dispersion of refractive index and characteristic energies such as oscillator strength E_o, (2.24-3.48eV) dispersion energy, E_d (8.1-22.3eV) and band gap energy, E_g (1.473 1.797eV) were obtained. An iterative method was used to fit a theoretical expressior to measured transmission data in the long wavelength region in which reasonably gooc results were obtained where absorption is negligible. The dispersion of the refractive index obtained from here were then analyzed using Wemple and Di Domenico's model where the oscillator strength, E_o and dispersion energy, E_d were subsequently obtained. Analysis of the effect of excess Te on the dispersion energy, E_d showed a lowering of this characteristic energy with density of excess Te (see Figure 4.17). This is due to the sensitivity of E_d to the density and structure of the films where in this case the presence of excess Te in the films introduces defects such as voids in the films which reduces the density of the films.

A blue shift in the absorption edge of the films was also observed in which the band gap, E_g was determined from the first derivative of the absorption spectrum. Good correlation however was not observed between the grain size calculated from Brus's electron confinement model with those obtained from XRD. The larger grain size of those obtained from XRD was thought to be due to clusters of smaller nanocrystallite. As for the question of the presence of a potential well needed to confine the carriers two models are proposed. In the first model the crystallites in the films are thought to be composed

of smaller nanocrystallites separated by grain boundaries. The segregation of impurities to the grain boundaries may create a sufficiently deep potential well to confine the charge carriers. In the second model crystallites are bounded by a thin layer of amorphous CdTe which has a larger band gap compared to crystalline CdTe. This is supported by the observation of a larger band gap in amorphous samples obtained in the current work.

D.C. electrical studies indicated two dominant conduction mechanisms in the films. The first is due to conduction in the extended states at high temperatures while the second is due to variable range hopping with a transition temperature of approximately 250K. Higher conductivity is also observed in the amorphous films which is presumably due to the relatively higher content of excess Te in the amorphous samples suggesting of more disorder in these films (Table 5.1). This is indeed the case where the parameter T_o (typical values of 10^7 in amorphous materials) obtained from the variable range hopping model showed higher values in the amorphous films. Determination of the magnitude of gap states from Schockley-Read's model of recombination showed values of 10^{13}-10^{19}cm^{-3} in the energy range of 0.6-0.3 eV above the valence band.

6.2. Suggestions for further work

Further work could be carried out to study the variation of the various structural, optical, electrical and electro-optical characteristics with the deposition conditions such as deposition rate, substrate temperature and impurities.

In the case of optical characterization low temperature measurements on the optical absorption could be carried out. This is especially useful in determining the existence of

quantum size effects since the presence of a peak in excitonic absorption would clearl identify the band gap. In addition modulation techniques such as electroabsorption an electroreflectance could be performed to clearly identify the energy at critical point $\nabla_k(E-E_o)=0$ in the band diagram.

As for electrical characterization, further study of a.c. conductivity and Hall effec measurement are needed. This will yield parameters such as hopping distance, mobilit and concentration of the charge carriers thus giving a more complete picture of the CdTe thin film characteristics.