CHAPTER 5 : CONCLUSION

5.1 Conclusion

Electron beam evaporation technique allowed the deposition and acquisition of good quality, polycrystalline CdTe thin films under the condition prescribed in table 3.1. The thin films exhibit properties of its own which deviates from the bulk properties of CdTe thin films.

Structural investigations revealed that all the CdTe thin films prepared in the present study are of polycrystalline nature with zinc blende structure. A preferred orientation of growth along the plane [111] was observed. The thin films obtained were formed by agglomeration of small nanoclusters as observed under SEM and TEM. The clusters are made of small nanocrystallites with sizes ranging from 30-110 nm. The sizes of crystallites were seen to increase with increasing film thickness. This indicates a preferential columnar growth of the nanocrystallites along the [111] plane direction. It can be concluded from the coherence and the adhesion of CdTe thin films to the substrate that they are physically connected. Moreover, the SEM photograph at high magnification showed the clusters immersed in a bed of small clusters indicating a complete physical interconnection between them.

A distribution in the crystallite size obtained were observed in the samples of the same batch, as shown in the figure 3.6 and also in the a single sample as seen under SEM. The distribution is seen to be skewed towards small crystallite size (~ 52%). Average cluster size obtained for deposition for 30 seconds under the condition mentioned in table 3.1 is 47.17 nm.

Thin films of CdTe prepared by this technique resulted in both compressive and tensile stress with the former dominating. This is evidenced by the compression and dilation in the lattice constant obtained. The compression, which is an expected phenomena in sputtered thin films is due to the 'peening' of sputtered atoms and molecules which were accelerated at high kV. The dilation is thought to be due to the presence of voids and also impurities in the sample. On the note that EDX analysis showed the presence of no other elements than Cd and Te, it was suggested that the presence of extra tellurium atoms in the films introduces a mismatch which results in the relaxation or dilation of lattice constant.

Lattice constant were also found to increase with the decreasing crystallite size, approaching a single crystal lattice constant value. At present, we only could say that this behavior is probably due the reduction in the compressive stress when the crystallite size is reduced thus result in the dilation of lattice constant.

Elemental analysis by EDX, showed the presence of high tellurium compared to cadmium in all the samples prepared. Tellurium was found to present in a ratio of 3:2 to Cadmium. The deviation from the stoichiometric ratio of 1:1 is may be due to the condensation of tellurium molecules (Te_2) at lower temperature (the deposition was carried out at 60°C) compared to cadmium. Moreover, tellurium has a high sticking coefficient towards adhesion to glass substrate compared to cadmium. Excess tellurium was suggested to have been incorporated in the formation of grain boundaries and may be present of a thin oxide layer, overlaying the thin film observed under SEM.

This was expected to influence the structural as well as the optical and electronic properties of CdTe thin films.

A deviation in the optical and electronic properties of electron beam evaporated CdTe thin films from the bulk properties were clearly seen as evidenced by the observed behavior of optical constants and the presence of a blue shift in the absorption edge.

Optical constants of CdTe thin films were determined from the transmittance spectra, using a method developed from the combination of methods proposed by Cisneros and Davis et.al. The methods can yield results with a standard deviation of less than 5 % in the high absorbing region while 8-10 % near and beyond the absorption edge.

A dispersion of refractive index was observed along the scanning region. The refractive index remains constant at low absorbing region (long wavelength limit) and increases near the absorption edge. All the films displayed similar behavior with an increase in the refractive index value with film thickness. This increase is due to the increase in the crystallinity, as evidenced by large grains in thick film, and continuity in the deposited thin films.

Dispersion of extinction coefficient, showed that the absorption takes place beyond λ = 850 nm and the absorption edge varied for films with varying thickness. This is correlated to the variation in the size of crystallite present in those films. Moreover, it was observed that thick films exhibiting high absorption compared to thin films.

Fundamental absorption edge was evaluated using the theoretical fitting of dipolar band-to-band transition and from the first derivative of optical density. It was found from the theoretical fitting, CdTe is a direct band gap material. These methods gave band gap at around 1.5 eV. Majority of the samples showed a blue shift in the absorption edge. The shift in the band gap is reasoned due to the crystallite size and to the presence of strain in the samples. As for that, the contribution in the shift of band gap by these factors were estimated.

The effect of crystallite size on the band gap shift was estimated using the Brus model while the effect of stress in the material was estimated using the approach used by Jimenez-Sandoval. It is seen that these two effects, contribute up to 60 % only to the band shift observed experimentally. As for the remaining 40 %, it is suggested that it may be due to the presence of amorphous phase in the thin films such as grain boundaries. Apart from that, the presence of free tellurium is also suspected to have an effect on the band shift.

Analysis of the results upto this point shows that layers of CdTe prepared by e-beam evaporation technique are made up of very small crystallites (20 - 50 nm, in radius) which they are physically well connected but electronically relatively isolated from each other as evidenced by quantum-size effect which requires electron localization to the respective crystallites. Leaving aside for the moment the question as to why this occurs, the implication in terms of electronic device behavior should be that any solid-state devices made using such layers will show a high resistance. Thus is borne out by the results on Al/CdTe junctions which gives a value for the resistivity of 10^6 - 10^8 Ωcm.

Returning to the absorption spectra (figure 4.9), the variation of E_g with crystallite size can show a number of effect on the shape of the spectra. The implication of a distribution of particle sizes (and therefore values of E_g) in the same layer is that the cut-off edge should be gradual rather than sharp. The fact that a fairly sharp cut-off obtained over a particular wavelength range suggests that one particle size is dominant as evidenced by the statistical distribution shown in figure 3.5. The sharpness of the curve near the maximum absorption (0.7 - 0.8 μm) varies from one sample to another suggesting large variation in crystallite size distribution from one sample to another.

The short-wavelength 'hump' on the absorption spectrum may be a partially resolved exciton peak; the fact that the 'hump' becomes increasingly prominent, suggest the reduction in crystallite size involved.

The shift in the spectra of samples prepared under same conditions to longer wavelength shows a logical consequence to the crystallite effect. Very small crystallites aggregation causes the blue shift.

To return to the question why these layers are made up of small crystallites which are physically connected and electronically isolated, few suggestions are given. First, the mechanism of deposition of CdTe which is based on the evaporation rate and the condensation rate of atoms, Cd, Te or molecules CdTe and Te_2. Tellurium which condenses at low temperature may form good grain boundaries to interconnect physically the CdTe crystallites.

The electronic isolation between the crystallites implies a potential barrier between them arising from the presence of a surface insulating layer. In the present analysis it is observed from EDX, tellurium which is an insulator present in high amount compared to cadmium in the films. This is expected to form a layer of insulator. Moreover it is expected a layer of oxide which could not be identified by EDX results may pose considerate effects on the electronic isolation of crystallites.

5.2 Suggestion for future work

As the polycrystalline films usually exhibit high resistivity when made contact, it is suggested some conditional deposition should be studied to prepare low resistivity CdTe thin films. It is expected, by varying the substrate temperature will reduce the resisitivity of the sample. The low resisitivity ($< 10^5\ \Omega$ cm) CdTe thin film will be suitable for the study of a.c. conductivity and Hall effect which will yield information on parameters such as hopping distance, mobility, charge carrier concentration and dielectric dispersion to complete the characterization of CdTe thin films.