CHAPTER 6

CONCLUSIONS AND SUGGESTIONS FOR FURTHER WORK

6.1 Conclusions:

The structural and optical properties of CdSe multilayer thin films are investigated in the present work. A total of 42 samples are identified and characterized by performing various experimental techniques. Probing the behaviour of these samples lead to evidences that support the presence of nanocrystallites and alter the property of the polycrystalline thin films. The results are summarized as follows.

(1) SEM pictures reveal that many samples are polycrystalline in nature as seen in the micrographs with bigger crystallites embedded in a matrix of fine grains. The crystallites are randomly oriented and their size is not uniform. Some samples have very fine grains while some have plain face, depicting the amorphous nature of the samples.

(2) Results from XRD show that some samples are polycrystalline and some are amorphous in nature. The polycrystalline films have cubic structure with a peak corresponding to the <111> plane orientation of zinc blende structure of CdSe. The percentage of deviation of the lattice contant of the film from its bulk single crystal value (3.51 Å) is

–1.9% to 1.2% and thus the unit cells have compressive as well as tensile stress. The crystallite size determined from the broadening effect of the peaks using Scherrer's equation vary from 4 to 28 nm.

(3) The thickness of the samples are determined using optical and Tolansky method. Thickness of films varies from 70 to 250 nm and a correlation is established between the above two methods.

(4) The value of refractive index in the long wavelength limit varies from 2.2 to 2.52 which is less than its bulk value of 2.55.

(5) Average value of the oscillator strength E_o and dispersion energy E_d calculated using single oscillator model are 3.22 eV and 19.9 eV respectively.

(6) The band gap energy E_g determined from transmission measurements varies from 1.71 to 2.36 eV. The maximum deviation from the bulk value of 1.66 eV is 0.70 eV, which is 42% higher than the bulk value.

(7) The blue shift in the band gap energy E_g is attributed to the quantum size effect and the radius of the clusters is calculated from the shift in energy of the film using the effective mass model proposed by Brus. The size of the crystallite varies from 4.4 to 22 nm.

(8) The energy shift ΔE of the band gap energy, depends on the reduced mass of electron- hole pair in a perfect crystal. This is found to be $0.109\ m_o$, where m_o is the rest mass of electron. Using the size of the crystallites determined from XRD measurements, the reduced mass μ of the electron-hole pair for the polycrystalline CdSe thin films is found to be $0.117\ m_o$, which is higher than its bulk reduced mass value. The

fundamental band gap value is found to be 1.765 eV compared to its bulk value of 1.661 eV.

6.2 Suggestions for further work:

Improvements can be made in the characterization techniques of the samples. Some enhancement will be beneficial in the method of preparation of the samples as it will improve the quality of the nanostructure film. Few of the suggestions are mentioned as follows.

(1) Transmission electron spectroscopy could be performed to know the structure of the crystallites deep inside the film.

(2) The samples could be annealed at various temperature and the variation in band gap energy and the crystallite size can be studied.

(3) The transmission spectroscopy of the samples could be taken at lower temperatures to confirm the existence of nanocrystallites as the excitonic peaks are more prominent at low temperatures.

(4) Samples could be prepared on heated substrates to improve the quality of nanostructured films.

(5) Samples could be prepared with uniform crystallite size by conducting optimization studies to improve the preparation methods.

(6) Techniques such as neutron activation analysis could be done to detect the impurities in the film as low as few parts per million.

(7) Electrical characterization of the samples could be carried out to find out the concentration of carrier charge density, which gives more information about the behaviour of samples.