CHAPTER VI
CONCLUSION AND FUTURE SCOPE
VI-1: CONCLUSION

In the present thesis few novel methods to control the morphology of blend films by spin coating method have been discussed. Chapter-I gives general information about the different type of solar cells, and a comparative study with the organic solar cells. Chapter-II gives information about the deposition methods, characterization techniques used in the work, cell fabrication method, and solar cell parameters and links between them. Details of the experimental work and the results have been discussed in chapters III, IV, and V.

In chapter-III, it is shown that the morphology of polymer-modified fullerene blends can be controlled by controlling the ambient during spin coating. The basic idea is that the phase separations in such blends depend upon the time it takes for the film to dry. It has been shown in this chapter that by purging an inert gas through the coating chamber or by introducing solvent vapor in the chamber the solvent evaporation rate during film drying process and hence the nanoscale phase separation between the blend components can be controlled. When the dry inert gas is purged through the chamber it quickly takes out the evaporated solvent and the film dries quickly. By controlling the gas flow rate through the chamber, drying time of the film can be altered. If the solvent is introduced into the chamber prior to film deposition, the chamber remains saturated with solvent vapor and thus it takes longer time for the film to dry. It has been shown that the nanoscale phase separation can be finely controlled.

Besides controlling the morphology by different experimental techniques, it is important to understand the basic phenomenon leading to phase separation which ultimately decides the nanoscale morphology. The inherent complexity of spin coating process and the need for material specific thermodynamic and kinetic parameters are the main modelling challenges. Therefore, a simple model which can provide quantitative information about the phase separated domains can have immense technological importance for rational design of processing conditions to achieve desirable morphology for various applications. In the later part of this chapter we have discussed the modeling results to explain the phase separation process by assuming the diffusion of PCBM once its solubility limit is crossed during the film drying process. To find the different parameters, we relied upon visual observation, as well as on the modeling the spin coating process. The Meyerhofer spin coating model was used for this purpose. To
calculate the diffusion of PCBM molecules Stroke-Einstein equation has been used. This is for the first time that, we have predicted the PCBM phase dimensions based on the number of molecules that can nucleate, before complete drying of the film. Simulation results matches closely with the experimental observations, and therefore it can be concluded that, assumption regarding the phase separation process is correct.

In chapter-IV, it is shown why a specific mixed solvent composition leads to appropriate film formation of composite (Polymer: Inorganic nanoparticle) during spin coating. As a typical case, P3HT: TiO$_2$ film formation have been discussed by taking chloroform as good solvent for P3HT while, ethanol, methanol and 2-propanol as solvents to disperse TiO$_2$ nanoparticles. For the formation of finely intermixed blend films, good solvents used for both the solute components must maintain a constant ratio throughout the drying process. If the content of any one solvent decreases in the course of film solidification larger aggregates of individual phases are obtained. By using the concept of Hansen solubility parameter, the effect of adding poor solvent in the P3HT solution in CF has been explained. Also the effect of nanoparticles on the solubility of polymer P3HT in the mixed solvent has been studied. Through simulation we have studied the solvent evaporation dynamics. It has been shown that, by knowing the evaporation rates of the component solvents and their HSP, exact quantities of mixed solvents required for appropriate film formation can be predicted through simulation. The film formation has been mainly explained by studying the solvent evaporation dynamics, and therefore this approach can be applied to suitable mixed solvent composition for any polymer-nanoparticle system. This study can provide a guideline for choosing mixed-solvent components and predict their specific ratio to form polymer-inorganic nanoparticle film with different degree of phase separation. In addition, it is shown that the rate of cooling of the polymer: nanoparticle blend after thermal annealing can be used to precisely control the nanoscale morphology of the individual phases. If the content of any one solvent, in the mixed solvent is less, finite solubility of the solute puts a limit on the film thickness. It has also been shown that coating multiple layers by spin coating, film thickness can be increased, in case it is limited by solubility of the solute components.

Synthesis of nanocrystalline TiO$_2$ powder has also been discussed in this chapter. However this powder was not dispersible in solvents like ET, MT, or 2P. Therefore this was not used for further studies.
In chapter V, annealing study of the P3HT:PCBM blend films was performed. It was concluded that the PCBM aggregation increases at the micrometer level with the annealing temperature and time. Initially PCBM dissolute into the P3HT matrix but, in the later stages aggregate formation dominates, and micrometer sized PCBM aggregates are formed at higher temperatures. This is in agreement with Ostwald ripening. The aggregates are formed due to the diffusion of PCBM spread around the nucleation centre. This in turn leads to decrease in PCBM from the bulk of the blend films. It was observed that purer phases are formed upon annealing only for longer annealing times at sufficiently high temperatures. Upon annealing for shorter times PCBM diffuses into the P3HT chains. Inspite of the diffusion of PCBM into the P3HT chains P3HT crystallinity was not affected. i.e. P3HT crystallinity can take place by local reordering of the chains, independently of whether PCBM diffuses out or diffuses in the P3HT chains. By studying the effect of titanium sub-oxide layer on the device performance, it was also found that the interface between the P3HT:PCBM layer and the titanium sub-oxide layer improves upon annealing. Maximum increase in device performance was observed upon annealing at 140°C. However upon annealing at 160°C degradation in device performance was observed. Similarly, upon annealing the blend after coating the titanium sub-oxide layer, results in improvement of device performance.

VI-2: FUTURE SCOPE

The present thesis gives novel experimental approaches to control the composite film morphology, and modelling study to understand the physics which leads to a particular phase separation. In chapter-III, morphology control by controlling the ambient during spin coating was demonstrated. This method can be used for other solvents like chloroform and di-chlorobenzene. Chloroform has a very high evaporation rate and therefore resultant blend film dries rapidly. As a result of this, components of the resultant blend film are mostly in amorphous state. By introducing the solvent vapor inside the chamber the film drying time can be increased and hence the crystallinity of the blend components can be enhanced. For solvents having an excessively low evaporation rate, film drying takes place too slowly, which can lead to the formation of excessively large aggregates of the blend components. Gas purging through the spin coating chamber can lead to rapid drying of the film, and therefore the resultant
morphology can be precisely controlled. The model given for PCBM aggregate formation during spin coating can be applied to other blend systems also. It can be checked whether this model can be applied to PCBM aggregate formation in blend films during thermal annealing.

In chapter-IV, mixed solvent approach was applied to form polymer-nanoparticle composite films of varying phase separation. This approach can be applied to completely new systems for the formation of newer composite films. Also a detail study to understand the device behavior described in the chapter needs to be undertaken.

In chapter-V, the effect of thermal annealing on the P3HT:PCBM blend films was explained. It was observed that upon thermal annealing dissolution of PCBM aggregates takes place initially and subsequently larger aggregates are formed. A detail modelling as well as experimental study to understand the degree of dissolution of the PCBM aggregates and the velocity of their aggregate formation can be undertaken.

To sum up, not only few novel experimental as well as modeling techniques were demonstrated in this thesis, but also it has opened up the scope to undertake few other challenging studies.