SUMMARY

Today, energy has become the lifeline and status symbol of civilized societies. All the nations have therefore focused their attention on renewable sources of energy. Solar energy is very attractive alternative source of energy. Solar cell is a device, which converts light energy received from sun directly into electrical energy. The application of solar energy is increasing day by day. The materials widely used for the fabrication of solar cells are; Si, GaAs, CdTe, CdSe, CdTe, CuS and CdS etc. Except Si all other materials by virtue of their electrical and optical properties must necessarily be in thin film form. Silicon is the most extensively used semiconductor in the fabrication of low cost terrestrial solar cells. Single crystal Si and GaAs solar cells are found to have efficiencies of the order of 18% and 20% respectively. In order to reduce the cost of fabrication of single crystal solar cells many workers have focused their attention towards polycrystalline silicon and Gallium Arsenide materials. PX-GaAs solar cells have high efficiency and lightweight as compared to PX-Si solar cells. These solar cells can also operate efficiently over a wide range of temperature and are more resistant to the radiation damages as compared to PX-Si solar cells.

The electrical and photovoltaic properties of PX-Si and PX-GaAs solar cells are greatly influenced by the grain-boundaries (GB’s), grain size, doping concentration, temperature, illumination level, intragrain defects and thickness of the device. It has been established that these properties are mainly controlled by the grain-boundaries. Several studies have shown that GB’s in these materials act as minority carrier recombination centers and majority carrier barriers. Whereas electrical and photovoltaic properties of PX-Si have been extensively
studied, only a few workers have investigated these properties of GaAs. This thesis is an endeavor to investigate the effect of grain size, GB states density, GB material, doping concentration, temperature and illumination level on the electrical and photovoltaic properties of PX-Si and PX-GaAs semiconductors. An effort is made to develop a comprehensive model of electrical conduction and carrier recombination at grain-boundaries, which is equally applicable to both the materials.

The thesis has been divided into seven chapters. Chapter-I is an introduction to polycrystalline semiconductors and physics of grain-boundaries. The next chapter is devoted to critical review of existing literature on electrical and photovoltaic properties of these materials and GB recombination processes under optical illumination. It is observed that, at present there is no suitable theoretical model, which can satisfactorily explain the effects of grain-boundaries on the electrical and photovoltaic properties of these materials. This fact has stimulated the author to formulate a comprehensive theory of carrier transport and carrier recombination at grain-boundaries in these materials.

In Chapter-III, a new model for electrical conduction across the GB’s of a PX-semiconductor in dark is proposed. According to this model carrier transport includes not only thermionic field emission through the GB space-charge potential barrier \(qV_g\)\(J_1\) component, thermionic emission over the barrier \(qV_g\) and then tunneling through the GB rectangular potential barrier \(q\phi\)\(J_2\) component, thermionic emission over these barriers \(J_3\) component but also two-step tunneling processes via the GB states \(J_4\) component. In contrast to the existing models for PX-Si, the present model is applicable to different dopant
species under small bias conditions. The author’s model is found to be valid over a wide doping concentration, temperature and grain size range.

Present work demonstrates that the height of the rectangular potential barrier $q\phi$ at GB is mainly related to the disordered nature of the GB material. The energy gap of the GB material is found to lie between the energy gap of single crystal Si and amorphous Si. The nature of this GB material is a function of dopant species, dopant density, dopant atoms segregation to the GB, temperature and annealing temperature. It is also found that the contribution of phonon scattering processes at the GB is insignificant as compared to that of the disordered nature of GB material. Author’s computation shows that in As-doped samples both As-clustering and dopant segregation mechanisms are present, whereas in Phosphorous-doped samples only dopant segregation mechanism is present. On the other hand, in Boron-doped samples no segregation and clustering mechanisms are present. Present thesis predicts that, below room temperature, in PX-Si the contribution of $J_4$ component to the total current density is more significant as compared to that of other components. It is also observed that whatever be the doping density at room temperature $J_2$ and $J_3$ components of current density are more significant than other components. The dependence of resistivity, carrier mobility and carrier concentration of PX-Si on doping density, dopant species, grain size and temperature is studied theoretically and these theoretical predictions are found to be in good agreement with the available experimental results.

In Chapter-IV, an effort is made to explain the electrical properties of PX-GaAs films by considering above mentioned conduction model. It is worthwhile to mention that the author’s conduction model is the first theoretical
model, which is applicable not only for PX-Si but also for PX-GaAs. A new relation has been proposed to explain the dopant segregation at the grain-boundsaries of PX-GaAs. It is observed that in n-type samples the dopant segregation mechanism is present whereas it is absent in p-type samples. It is seen that in these two materials the contribution of each component of current flowing across the GB is widely different from each other. For example, in PX-GaAs the contribution of $J_4$ component is always very significant as compared to other components especially in high doping density range. This type of behaviour of $J_4$ component is not observed in PX-Si.

Present study demonstrates that the dependence of $q\phi$ on doping density is different for PX-GaAs and PX-Si. However the dependence of $q\phi$ on temperature is same for two materials. It is found to decrease with decrease in temperature. This fact demonstrates that the barrier $q\phi$ is related with the disordered nature of GB material. Present theory shows that the electrical properties of PX-GaAs are controlled by $J_1$ and $J_4$ components of current in very low temperature range. This fact predicts that TST mechanism of carrier transport is very important in PX-GaAs films especially in low temperature range.

The recombination processes and carrier transport across the GB in PX-Si and PX-GaAs under optical illumination are studied in Chapter-V. Author’s recombination model is based on the assumptions of Gaussian energy distribution of midgap GB interface states. Author’s study is valid at sufficient illumination levels, for partially depleted grains and over a wide temperature range. Present analysis predicts that $qV_g$ decreases with increasing illumination level and grain size. However in the large grain size ranges the dependence of $qV_g$ on grain size decreases. It is observed that the dependence of $J_t(W_g)$
(recombination current density at depletion region) and \( S(o) \) (recombination velocity at the GB) on grain size and illumination level for these two materials is different from each other especially in the large and small grain size ranges. It is also found that the magnitude of \( J_r(W_g) \) in PX-GaAs is much larger than that in PX-Si. Therefore, the recombination of minority carriers in the depletion region at GB cannot be neglected in GaAs. On the other hand recombination current density \( J_r(o) \) increases with increasing grain size and attains a maximum and becomes constant at very large grain sizes for the two materials.

In this Chapter the effect of optical illumination, grain size, temperature and GB scattering on the resistivity and mobility in PX-semiconductor materials under optical illumination is also studied by using above mentioned electrical conduction model. It is found that as the temperature decreases the contribution of all the components of current density except \( J_3 \) increases. At low temperatures, the electrical conduction in both the materials is mainly controlled by \( J_2, J_3 \) and \( J_4 \) components. As observed in dark condition the potential barrier \( q\phi \) is found to decrease with decreasing temperature under optical illumination. Computations show that the dependence of effective carrier mobility \( \mu^* \) in these materials on temperature is different in different temperature ranges. At low temperatures and high illumination levels \( qV_g \) is very small as compared to \( q\phi \). As a result of this resistivity and carrier mobility in these materials is controlled by GB scattering effects. A good agreement between computed results and experimental data demonstrates that author's conduction model for PX-semiconductor material is valid not only in dark but also under optical illumination.
A new relation for effective diffusion length $L^*$ of minority carriers in PX-semiconductors has been developed in Chapter-VI. It is predicted that in very small grain size range $L^*$ is controlled by the GB recombination processes and GB recombination in junction space-charge region of a solar cell. The effect of vertical grain-boundaries present in the junction space-charge region on the effective lifetime is also discussed. Under sufficient illumination levels this model is valid for all partially depleted grains with base doping levels smaller than $5 \times 10^{18} \text{ cm}^{-3}$. Author has demonstrated that the GB recombination and the present effective diffusion length models are applicable not only to p-n junction solar cell but also to MIS/SIS solar cells. It is found that at $d << L_b$, solar cell parameters decrease rapidly with decreasing grain size. The agreement between computed and available experimental data predicts that the effects of vertical grain-boundaries in the junction space-charge region should not be neglected in order to study the performance of PX-Si solar cells. Author has also shown that the reverse saturation current density ($J_{o2L}$) in the junction space charge region is controlled by the effective lifetime component $\tau_{gd}$ instead of the effective lifetime $\tau_{n^*}$. In contrast this concept is not considered by any of the existing models.

In this Chapter, author has also studied the dependence of MIS/SIS PX-Si solar cell parameters on the thickness of the insulator layer and the grain size. It is found that minority carriers quasi-Fermi level at the semiconductor surface $E_{FP}(o)$ depends on oxide layer thickness $\delta$ and grain size together with other factors. A good agreement between the computed results and the available experimental data for all values of grain size ($W_g < d$) predicts that the shrinkage
of Schottky barrier and variation of minority carrier mobility with grain size are negligible.

The electrical properties and performance of solar cells fabricated on PX-GaAs films are studied in Chapter-VII by considering the GB recombination model proposed in Chapter-V and the model for effective diffusion length developed in Chapter-VI. Present computations show that in very small grain size range the diffusion length of minority carriers in PX-GaAs solar cells is controlled not only by GB recombination processes but also by the GB recombination in junction space-charge region. A similar behavior of L* is observed for PX-Si solar cells. Author’s calculations show that reverse saturation currents are much smaller for PX-GaAs than those for PX-Si solar cells. In these films, J_{o2L} is found to be much larger than J_{o1L} for all grain sizes. The most important prediction of the present work is that the efficiency of GaAs solar cells is very sensitive to the grain size in the very small grain size range as compared to that observed for PX-Si solar cells.

In order to explain the performance of PX-GaAs MIS solar cells author modified the expression for short circuit current density J_{sc} of PX-Si MIS/SIS solar cells and demonstrated that for PX-GaAs solar cells recombination of minority-carriers at I-S interface and in the junction region is much more appreciable as compared to that observed in PX-Si MIS solar cells. It is also shown that the diode quality factor n_2 is independent of grain size in PX-GaAs solar cells but this parameter varies with grain size for PX-Si solar cells.

Good agreement is found between predictions of this thesis and the available experimental data. The qualitative features of the present work can be applicable to any other polycrystalline material / thin film.