Effect of grain boundaries on photovoltaic properties of PX-GaAs films

M K Sharma & D P Joshi*
Principal, Govt Sr Sec School Kolar, Sirmour (H P)
*Department of Physics, D B S (P G) College, Dehradun
E-mail: dr.manojsharma266@rediffmail.com; *dpj55@rediffmail.com
Received 23 September 2009; revised 21 January 2010

A new relation for the effective diffusion length of minority carriers has been presented and the performance of polycrystalline GaAs solar cells has been studied theoretically. It has been found that in the very small grain size range, the diffusion length of minority carriers in these devices is controlled not only by the grain boundary (GB) recombination processes but also by the GB recombination processes in the junction space charge region. In the very small grain size range, the efficiency of these solar cells has been found to be very sensitive to the grain size as compared to that observed for PX-Si solar cells. A good agreement has been found between the theoretical predictions and the available experimental data.

Keywords: Photovoltaic properties, GaAs solar cells, PX-GaAs films

1 Introduction

Direct band gap semiconductors are best suited for fabrication of high efficiency thin film photovoltaic devices due to their sharp absorption edges and large optical absorption coefficients. For direct band gap materials, the minority-carrier diffusion-length and grain size requirements are less stringent than those for the indirect band gap materials.

The potential importance of low cost polycrystalline films of GaAs for solar cells has been studied by many researchers. In the past, less attention was given to the research work on devices related to GaAs due to low availability of this material. However, in recent years, the research work on PX-GaAs material has increased rapidly due to the wide application of this material in microwave and optoelectronic devices.

The presence of two elements and the factor of stoichiometry make the study of GaAs much more difficult than of widely studied PX-silicon. As a result of this, only a few researchers have studied the influence of grain boundaries on the electrical and photovoltaic properties of PX-GaAs material\(^1\). In the present work a relation for the effective diffusion length of minority carriers (\(L_n^*\)) is developed and the variation of PX-GaAs solar cells parameters with grain size is studied by considering Gaussian energy distribution of grain boundary states\(^2\), and recombination of minority carriers in the grain boundary and junction depletion regions of the solar cells.

2 Theory and Discussion

2.1 Recombination velocity near the GB region

The electrical properties\(^2\) of PX-GaAs films have been studied and shown in Fig. 1 by considering the following Gaussian energy distribution of GB states:

\[ N_{gs}(E) = N_{gs} \exp\left[\frac{-(E-E_t)^2}{2S^2}\right] \left(\sqrt{\frac{2}{\pi}} S\right) \quad \text{(1)} \]

where \(N_{gs}\) is the total density of localized states per unit area, \(S\) is the distribution parameter and \(E_t\) is the energy position of the mean value of interface states from the valance band edge. PX-semiconductor transport properties are assumed as one dimensional. Further it has been assumed that this material consists of identical columnar grains of cross-sectional area \(d^2\) and length \(H\) (base thickness), and all GB states have equal capture cross-sections.

Under optical illumination, the photogenerated minority carriers recombine with the trapped majority carriers at the grain boundary and a new interface charge is established at the grain boundary through S-R-H capture and emission processes. This in turn reduces the grain boundary (GB) barrier height from its dark value and the Fermi level splits into electron and hole quasi Fermi levels \(E_{Fn}\) and \(E_{Fp}\), respectively (Fig. 1). By equating the total charge accumulated in the GB interface states to the charge in the two neighbouring depletion regions, one can obtain \(qV_g\) under optical illumination:
2.2 Effective lifetime and diffusion length of minority carriers

Various approaches have been suggested for assigning effective minority carrier lifetime (\(\tau_n^e\)), all based on different assumptions concerning GB properties and geometry.\(^4,6\) The effective lifetime of minority carriers in the base region of PX-solar cells is expressed by:

\[
\frac{1}{\tau_n^e} = \frac{1}{\tau_b} + \frac{1}{\tau_{ng}} \quad \text{…(7)}
\]

where \(\tau_b\) is the bulk lifetime of minority carriers and \(\tau_{ng}\) is the surface component of minority carrier lifetime. Considering \(W_g\) as the electrical width of GB and using the concept of effective recombination velocity, many researchers\(^1,5\) have expressed the following expression for \(\tau_{ng}\):

\[
\tau_{ng} = W_g / S(W_g) \quad \text{…(8)}
\]

However present computations show that the effective recombination velocity \(S(W_g)\) depends on the grain size. Its value is much greater than that of \(S(o)\) in the small grain size range but this is not true for large grain sizes. As a result of this, minority carrier diffusion length \(L_n\) or lifetime cannot remain constant in the GB depletion region. This fact predicts that the electrical width of a GB should not be represented by \(W_g\) (as has been done in the various existing studies\(^1\)) but by \(L_n\).

Considering this approach the following empirical relations for \(\tau_n^e\) in the base region of a PX-GaAs solar cell are proposed in the present study.

\[
\tau_{ng} = f W_g d/2 \, S(W_g) \, L_n \quad \text{…(9)}
\]

where \(f\) is a fitting parameter. Its value is different for different materials. For PX-GaAs material \(f = 24\). Considering the relation between lifetime and diffusion length of electrons in p-GaAs, the Eq. (9) can be expressed as:

\[
\tau_{ng} = [f W_g d/2 \, S(W_g)]^{2/3} \, (D_o)^{-1/3} \quad \text{…(10)}
\]

In the present work only columnar grains are considered. It is clear that a part of the vertical grain boundary also lies in the junction depletion region. Therefore, GB recombination effects in the junction depletion region must be considered. It is clear that a part of the vertical grain boundary also lies in the junction depletion region. Therefore, GB recombination effects in the junction depletion region must be considered. It is clear that a part of the vertical grain boundary also lies in the junction depletion region. Therefore, GB recombination effects in the junction depletion region must be considered. It is clear that a part of the vertical grain boundary also lies in the junction depletion region. Therefore, GB recombination effects in the junction depletion region must be considered.
where \( W_b \) is junction width in the base region of a solar cell.

If the base doping level is greater than \( 10^{17} \text{ cm}^{-3} \), then the Auger recombination processes and band gap narrowing effects become significant\(^7\). Auger lifetime \( \tau_{nA} \) decreases rapidly on increasing doping density. Under this condition, the effective lifetime of minority carriers in the base region of the PX-solar cells is:

\[
\frac{1}{\tau_{n}^*} = \frac{1}{\tau_n} + \frac{1}{\tau_{ng}} + \frac{1}{\tau_{nj}} + \frac{1}{\tau_{nA}}, \quad \ldots(12)
\]

where \( \tau_{nA} = \frac{1}{(C_n N_A)^2} \), \( C_n = 10^{-31} \text{ cm}^6 \text{s} \) is the band to band Auger recombination coefficient\(^8\), and \( N_A \) is the base doping density. The effective diffusion length of minority carriers \( L_n^* \) in these devices can be expressed as:

\[
L_n^* = (D_n \tau_n^*)^{1/2} \quad \ldots(13)
\]

where \( D_n \) is diffusion constant of the electrons. Similarly the effective lifetime of minority carriers in the emitter region of the solar cell is given by:

\[
\frac{1}{\tau_{p}^*} = \frac{1}{\tau_p} + \frac{1}{\tau_{pg}} + \frac{1}{\tau_{dp}} + \frac{1}{\tau_{pA}}, \quad \ldots(14)
\]

where the minority carrier lifetime in the “dead layer” (which is believed to exist adjacent to the top region of the \( n-p \) solar cell) \( \tau_{dp} \) is found\(^9\) to be about 3ns, and \( \tau_{pA} \approx \frac{1}{(C_N N_D)^2} \). Here \( C_N = 2.8 \times 10^{-31} \text{ cm}^6 \text{s} \) and \( N_D \) is doping density in the emitter region.

To make the study of the physics of GB recombination simpler, uniform photogeneration of electrons and holes throughout the volume of the specimen are assumed. The computed variation of \( qV_g \) as a function optical illumination level and grain size is shown in Fig. 2. The values of the parameters used are listed in Table 1. The values of different selected parameters are reasonable and agree with several studies. These plots show that as illumination level increases \( qV_g \) decreases. It is also observed that in the low illumination level the dependence of \( qV_g \) on illumination level for PX-GaAs is more as compared to PX-Si (Ref. 3). In contrast, in the large grain size range the dependence of \( qV_g \) on grain size of these devices is less as compared to that of PX-Si because in this range, quasi-Fermi level splitting is independent of grain size for PX-GaAs devices.

The variation of \( \tau_{n}^* \) with grain size for PX-GaAs solar cell under AM1 optical illumination is shown in Fig. 3 by considering the parameters given in Table 1.
Computations show that in the small grain size range ($d << L_b$), $\tau_n^*$ is mainly controlled by the component $\tau_{nj}$. Figure 4 shows the computed variation of effective diffusion length as a function of grain size. It is found that in the very large grain size range, $L_n^*$ is approximately independent of $d$ because in this range bulk recombination is the dominant process. As grain size decreases the effect of GB recombination processes increases and hence $L_n^*$ becomes approximately proportional to the grain size. In the very small grain size range ($d << L_b$), $L_n^*$ is controlled by the GB recombination in the junction space charge region of the solar cell. This variation demonstrates that in the very small grain size range the behaviour of GBs of PX-GaAs and PX-Si materials are different.

2.3.1 Short circuit current density

Considering the above concept of effective diffusion length of minority carriers and using one-dimensional theory of single-crystal $n^+ - p$ junction solar cell, the short circuit photocurrent density for the $n^+ - p$ PX-GaAs solar cell is given by:

$$J_{sc} = J_n + J_{dr} + J_p$$

where $J_n$, $J_{dr}$, and $J_p$ are the photocurrent density due to electrons collected from the undepleted part of the base region, photocurrent density resulting from the carrier generation in the depleted part and photocurrent density due to charges collected from the top region of the $n^+ - p$ junction solar cell, respectively. These components of $J_{sc}$ are expressed by:

$$J_n = \sum_{\lambda} q \alpha F(\lambda) \exp[-\alpha(x_j + W_b)]$$

$$\{[\alpha(1/L_n^*+1)-1] - \exp(-H/L_n^*) - \exp(-\alpha H^*)\}$$

and

$$J_p = \sum_{\lambda} q MF(\lambda) \exp(-\alpha x_j)\{1-\exp(-\alpha W_b)\}$$

where $M = \tau_n^*/\tau$ and $\tau$ is the transit time for carriers crossing the depletion layer.

$$\tau = W_b^2/\mu_n V_b$$

and $F(\lambda)$ is the number of photons incident per cm$^2$ per second per unit band width at wavelength $\lambda$, $x_j$ is the junction depth and $H'$ is the thickness of the base region, $S_p$ is the recombination velocity of the holes at the top region, $L_p^*$ is the effective diffusion length of holes in the emitter region and $V_b$ is the junction space-charge potential barrier height. Present study shows that $M = 1$. 

Fig. 3 — Variation of effective lifetime $\tau_n^*$ for PX-GaAs solar cell for various grain sizes

Fig. 4 — Variation of effective diffusion length $L_n^*$ with grain sizes; the experimental points are taken from Refs 3, 10, 11, 13, 14
Figure 5 represents the computed variation of $J_{sc}$ with grain size at AM1 illumination level. A good agreement is observed between the theoretical results and available experimental data\textsuperscript{3,10,11,13,14}. It is also observed that in very small grain size range $d < L_b$, the dependence of $J_{sc}$ on grain size is much greater than that in the large grain size range. This demonstrates that in very small grain size range $J_{sc}$ is not only controlled by the GB recombination processes but also by the GB recombination processes in the junction space-charge region.

It is worthwhile to mention that the present work does not consider the variation of minority carrier mobility ($\mu_n$) with grain size and the shrinkage of junction barrier height under optical illumination as has been done in Ghosh et al.\textsuperscript{5} study.

2.3.2 Open circuit voltage

The open circuit voltage of an ideal solar cell is computed by the following expression

$$J_{oc} = J_{oc1} \{\exp(qV_{oc}/kT) - 1\} + J_{oc2} \{\exp(qV_{oc}/n_2 kT) - 1\}$$

...(20)

where the first term represents the diffusion current density and the second term represents the space charge recombination current density under illumination. Here $J_{oc1}$ and $J_{oc2}$ are the corresponding reverse saturation current densities and $n_2$ is diode quality factor.

Figure 6 represents the variation of open circuit voltage $V_{oc}$ with the grain size for this device. It is again seen that $V_{oc}$ is very sensitive to the grain size in the small grain size range ($d < L_b$). Present theoretical predictions are in good agreement with the available experimental data\textsuperscript{3,10,11,13,14}. We further note that in this material $V_{oc}$ is mainly controlled by the space-charge recombination current density. The dependence of $V_{oc}$ on this current density increases as grain size decreases. As a result of this, the diode quality factor $n_2$ is found to be approximately independent of grain size for this material. On the other hand, $n_2$ is found to be varying with grain size in case of PX-Si solar cell\textsuperscript{3}.

2.3.3 Efficiency

Figure 7 represents the variation of $\eta \%$ with grain size under AM1 illumination. A good agreement is obtained between theoretical predictions and available experimental results\textsuperscript{3,10,14-16}. By assuming 10% loss in efficiency and following empirical relation for the fill factor\textsuperscript{16}:

$$FF = FF_o (1 - 1.5r) + r^2/8.4$$

...(21)

where $r = R_s' J_{sc}/V_{oc}$, $FF_o$ is ideal curve factor in the absence of series resistance and $R_s' = 2.2$ ohm-cm\textsuperscript{2}. It is found that the efficiency of these devices is very sensitive to grain size in the very small grain size range. It is also observed that as grain size increases the dependence of efficiency on grain size decreases. The present study demonstrates that theoretical propositions of PX-GaAs thin films can also be
explained by Gaussian distribution model of GB states. The importance of Gaussian distribution of GB interface states is also underlined in a recent study.  

3 Conclusions

A new relation for the effective diffusion length of minority carriers is proposed and the dependence of PX-GaAs solar cell’s parameters on grain size is studied. The main predictions of the present work are: In the very small grain size range, the diffusion length of minority carriers in PX-GaAs solar cells is controlled not only by the GB recombination processes but also by the GB recombination in junction space-charge region; the efficiency of these solar cells is very sensitive to grain size in very small grain size range as compared to that observed for PX-Si solar cells, and the diode quality factor $n_2$ is found to be independent of grain size. On the other hand, in PX-Si solar cells, this parameter is found to vary with grain size.

Though the present analysis is carried out for polycrystalline GaAs, the qualitative features of this work are applicable to any polycrystalline material/thin film having columnar grains.

References