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

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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 stochiometry 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:

$$N_{gs}(E) = N_{gs}\exp[-(E-E_t)^2/2S^2]/(\sqrt{2\pi}\,S) \qquad \ldots(1)$$

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:

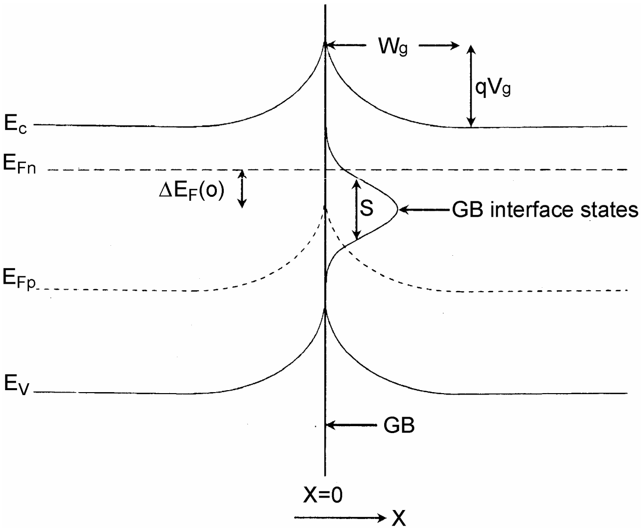

Fig. 1 — Energy band diagram of *n*-type polycrystalline GaAs under optical illumination

$$(8\varepsilon N_A qV_g)^{1/2} = q \int_{E_v(o)}^{E_c(o)} N_{gs}(E) f(E)\, dE, \qquad \ldots(2)$$

where the permittivity of PX material is ε and N_A is the doping density. The occupation function $f(E)$ is given by:

$$f(E) = [\sigma\, n(o) + \sigma_c n_i \beta^{-1}]/[\sigma_N n(o) + \sigma_N n_i \beta + \sigma_c\, p(o) + \sigma_c n_i \beta^{-1}] \qquad \ldots(3)$$

where $n(o)$ and $p(o)$ are electron and hole densities at the GB, respectively, n_i is intrinsic carrier concentration, $\beta = \exp[(E-E_i)/kT]$, and E_i is the intrinsic Fermi level. The electron and hole concentrations at the GB are given by :

$$n(o) = N_A \exp(-qV_g/kT) \qquad \ldots(4)$$

$$p(o) = (n_i^2/N_A)\exp(qV_g/kT)\exp(\Delta E_F(o)/kT) \qquad \ldots(5)$$

where $\Delta E_F(o) = E_{Fn}(o) - E_{Fp}(o)$ is the separation of quasi-Fermi levels at the grain-boundary.

For PX semiconductors there are two recombination velocities of minority carriers namely the surface recombination velocity at the grain boundary defined $S(o)$ and effective recombination velocity at the depletion edge $S(W_g)$ defined by the following relation:

$$S(W_g) = J_r(o)/(2qP(W_g)) \qquad \ldots(6)$$

where $P(W_g)$ is the minority-carrier density at the grain boundary depletion edge and $J_r(o)$ is the GB recombination current density at the GB surface[3].

2.2 Effective lifetime and diffusion length of minority carriers

Various approaches have been suggested for assigning effective minority carrier lifetime (τ_n^*), 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:

$$1/\tau_n^* = 1/\tau_b + 1/\tau_{ng} \qquad \ldots(7)$$

where τ_b is the bulk lifetime of minority carriers and τ_{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[4,5] have expressed the following expression for τ_{ng}:

$$\tau_{ng} = W_g/S(W_g) \qquad \ldots(8)$$

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 τ_n^* in the base region of a PX-GaAs solar cell are proposed in the present study.

$$\tau_{ng} = f\, W_g\, d/2\, S(W_g)\, L_n \qquad \ldots(9)$$

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:

$$\tau_{ng} = [f\, W_g\, d/2\, S(W_g)]^{2/3} (D_n)^{-1/3} \qquad \ldots(10)$$

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[6]. The vertical GB recombination in the junction depletion region of a PX-GaAs can be represented by the following empirical relation:

$$\tau_{nj} = W_b / S(W_g) \qquad \ldots(11)$$

where W_b is junction width in the base region of a solar cell.

If the base doping level is greater than 10^{17} cm^{-3}, then the Auger recombination processes and band gap narrowing effects become significant[7]. Auger lifetime τ_{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:

$$1/\tau_n^* = 1/\tau_b + 1/\tau_{ng} + 1/\tau_{nj} + 1/\tau_{nA}, \qquad \ldots(12)$$

where $\tau_{nA} = 1/[C_p N_A^2]$, $C_p = 10^{-31}$ cm^{6}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:

$$L_n^* = (D_n \tau_n^*)^{1/2} \qquad \ldots(13)$$

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:

$$1/\tau_p^* = 1/\tau_b + 1/\tau_{pg} + 1/\tau_{dp} + 1/\tau_{pA}, \qquad \ldots(14)$$

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) τ_{dp} is found[9] to be about 3ns, and $\tau_{pA} \approx 1/[C_N N_D^2]$. Here $C_N = 2.8\times10^{-31}$ cm^{6}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 τ_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.

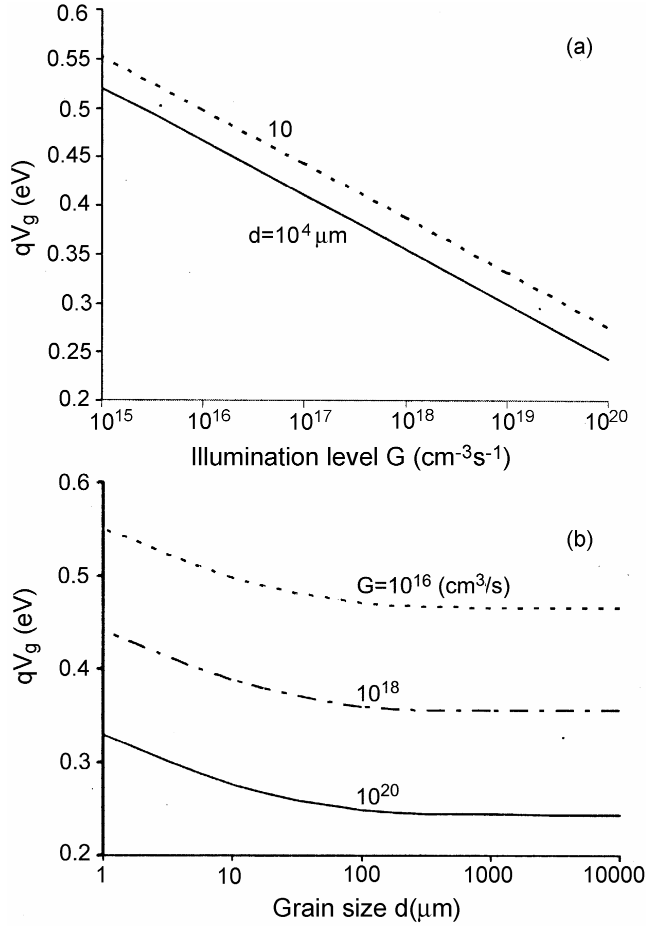

Fig. 2 — (a) Variation of GB potential barrier with illumination level at different grain sizes; (b) Variation of GB potential barrier with grain sizes at different illumination levels

Table 1 — Parameter values used in the calculations of PX-GaAs solar cells

Parameters	Values	Parameters	Values
N_{gs}(cm^{-2})	1.2×10^{12}	σ_c(cm^2)	10^{-13}
N (cm^{-3})	5×10^{16}	σ_N(cm^2)	8×10^{-15}
E_t (eV)	0.36	T (K)	300
L_b (μm)	6	H (μm)	50
τ_b (s)	3.47×10^{-9}	V_{th} (cm^2/s)	10^7
L_p (μm)	4	V_b (eV)	0.8
τ_p (s)	3×10^{-9}	x_j (cm)	2×10^{-5}
D_n (cm^{2}s^{-1})	103.6	R_s' (Ω-cm^2)	2.2
D$_p$ (cm^{2}s^{-1})	6.475	ε (F/cm)	1.16×10^{-12}
μ_n (cm^2/V-s)	4000	S_p (cm/s)	10^4
μ_p (cm^2/V-s)	250	n_2	2
E_g (eV)	1.42		
G (1 sun = cm^{-3}/s)	3×10^{19}		
S (eV)	5kT		

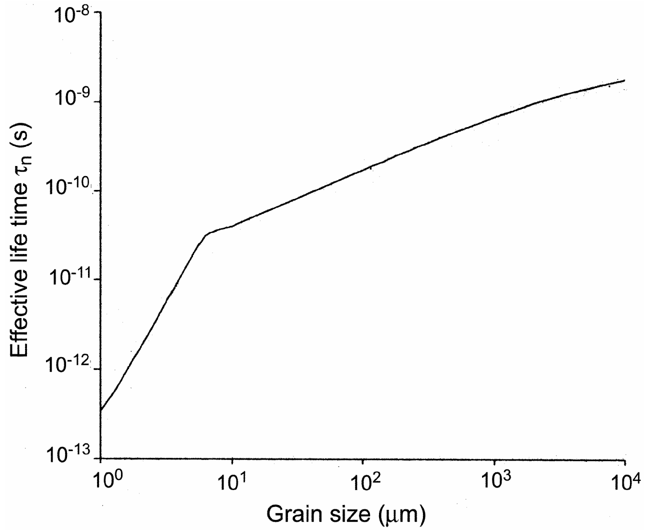

Fig. 3 — Variation of effective lifetime τ_n^* for PX-GaAs solar cell for various grain sizes

Computations show that in the small grain size range ($d \ll L_b$), τ_n^* is mainly controlled by the component τ_{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 ($d \ll L_b$), 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[3].

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 :

$$J_{sc} = J_n + J_{dr} + J_p \qquad \ldots(15)$$

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:

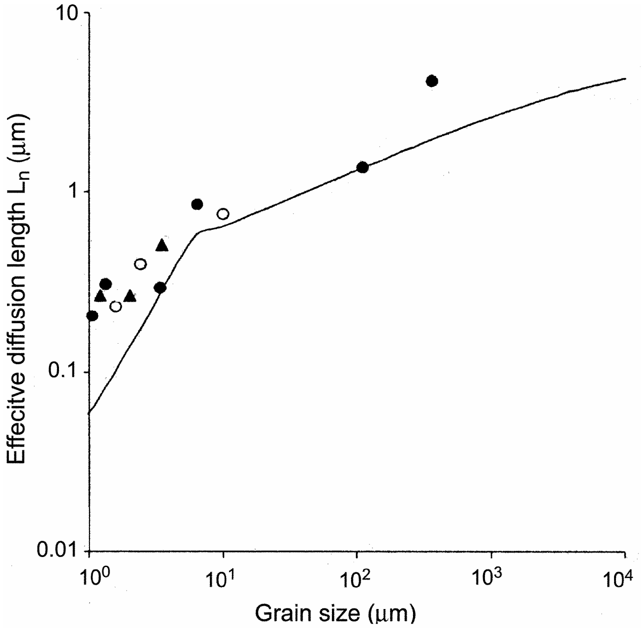

Fig. 4 — Variation of effective diffusion length L_n^* with grain sizes; the experimental points are taken from Refs 3, 10, 11, 13, 14

$$J_n = \sum_{\lambda} q\, \alpha\, F(\lambda)\, exp[-\alpha(x_j + W_b)] \{(\alpha + 1/L_n^*)-1 - [\exp(-H'/L_n^*) - \exp(-\alpha H')] [L_n^*(\alpha^2 - H'/L_n^{*2}) \sinh(H'/L_n^*)]^{-1}\} \qquad \ldots(16)$$

$$J_{dr} = \sum_{\lambda} qMF(\lambda) \exp(-\alpha x_j)\{1-\exp(-\alpha W_b)\} \qquad \ldots(17)$$

and

$$J_p = \sum_{\lambda} q\alpha F(\lambda) L_p^*(\alpha^2 L_p^{*2}-1)^{-1}\{[(S_p L_p^*/D_p)+\alpha L_p^* -\exp(-\alpha x_j)\{(S_p L_p^*/D_p)\cosh(x_j/L_p^*) + \sinh(x_j/L_p^*)\}][(S_p L_p^*/D_p)\sinh(x_j/L_p^*) +\cosh(x_j/L_p^*)]^{-1} -\alpha L_p^* \exp(-\alpha x_j) \qquad \ldots(18)$$

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

$$\tau = W_b^2/(V_b\, \mu_n) \qquad \ldots(19)$$

and $F(\lambda)$ is the number of photons incident per cm^2 per second per unit band width at wavelength λ, 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 $M = 1$.

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[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 (μ_n) with grain size and the shrinkage of junction barrier height under optical illumination as has been done in Ghosh *et al.*[5]study.

2.3.2 Open circuit voltage

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

$$J_{sc} = J_{o1L}\{\exp(qV_{oc}/kT)-1\} + J_{o2L}\{\exp(qV_{oc}/n_2kT)-1\} \quad \ldots(20)$$

where the first term represents the diffusion current density and the second term represents the space charge recombination current density under illumination. Here J_{o1L} and J_{o2L} 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[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[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[3,10,14-16]. By assuming 10% loss in efficiency and following empirical relation for the fill factor[16]:

$$FF = FF_o\,(1-1.5r) + r^2/8.4 \quad \ldots(21)$$

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^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

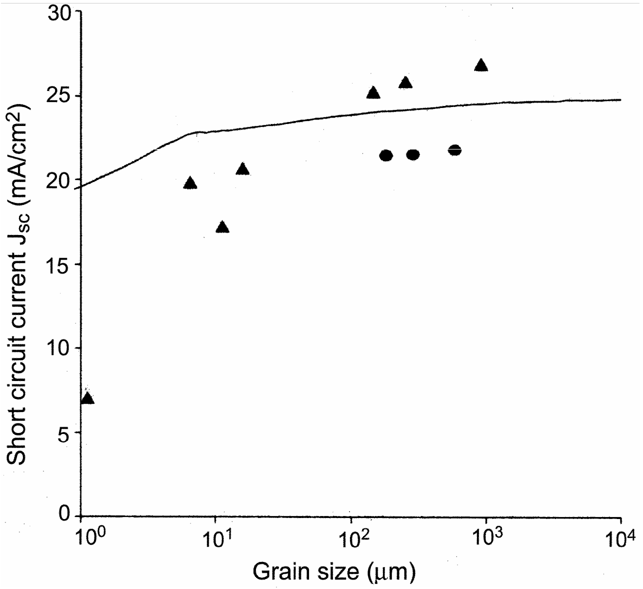

Fig. 5 — Variation of short-circuit current density with grain size; the experimental points are taken from Refs 3, 10, 11, 13, 14

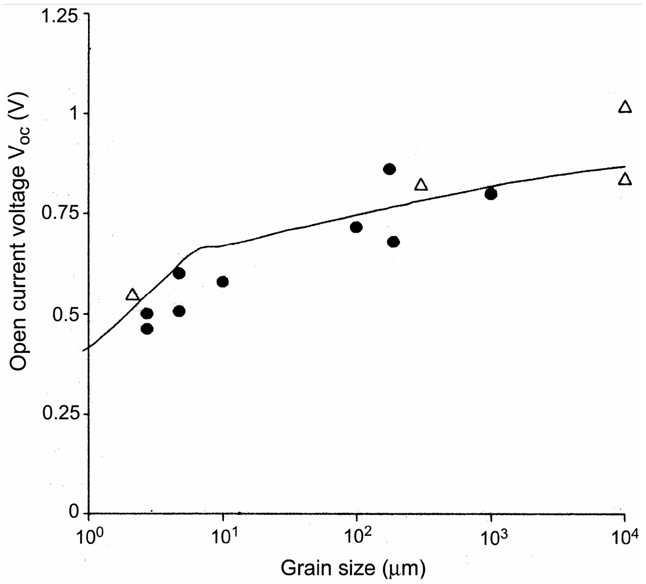

Fig. 6 — Variation of open circuit voltage with grain size; the experimental points are taken from Refs 3, 10, 11,13,14

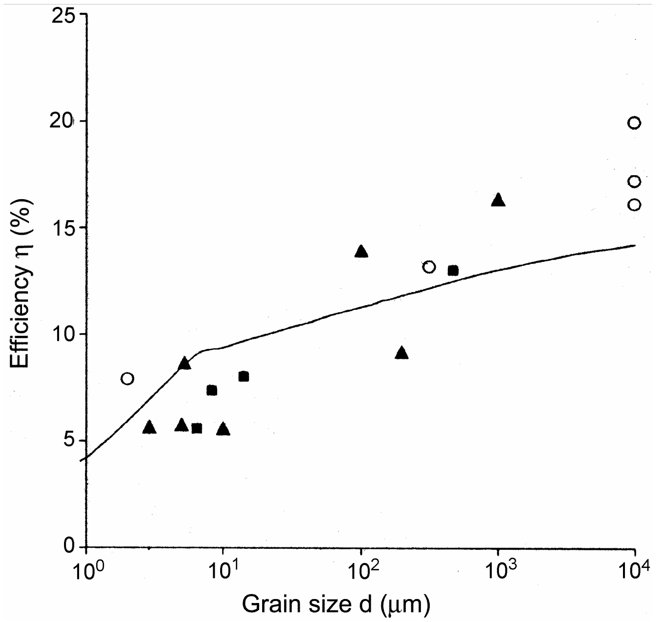

Fig. 7 — Variation of efficiency with grain size; the experimental points are taken from Refs 3, 10, 14-16

explained by Gaussian distribution model of GB states. The importance of Gaussian distribution of GB interface states is also underlined in a recent study[17].

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.

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