Short circuit current variation of CIGS solar cells with grain boundaries recombination velocity

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Received 10 June 2003; revised 18 August 2004; accepted 16 September 2004

The material CuIn$_x$Ga$_{1-x}$Se$_2$ (CIGS with 0$<x<0.3$) has attracted much attention, recently, all over the world as a prospective material for photovoltaic application. The addition of gallium in CIS (CuInSe$_2$) considerably improves not only the performance but the stability and efficiency of the device also. A theoretical analysis of variation of short circuit current density ($J_{SC}$) of polycrystalline solar cell has been reported. As the grain size ($d_G$) and grain boundary recombination velocity ($S_{GB}$) play an important role in deciding device characteristics, the calculations of the dependence of short-circuits photocurrent density ($J_{SC}$) have been done on these parameters. The results show a good agreement with the experimental results. A small discrepancy may be attributed to the fact that the typical shape of the grains was assumed to be square-face columnar shaped.

[Keyword: Grain boundaries, Recombination velocity, Grain size, Short circuit current density, CIGS solar cells]

IPC Code: H 01 L 31/0272

1 Introduction

A number of ternary semiconductors of the type I-III-VI, which crystallize in the chalcopyrite structure, have attracted considerable interest because of their potential use for solar cell applications. The most thoroughly studied material is CIS and it has been established that the electrical and optical properties of this compound are dominated by the presence of intrinsic defects such as vacancies, interstitials and antisite defects. Recent developments have improved the performance of thin film solar cells to the efficiencies of about 12%, which is however still well below their potential maximum efficiencies. Besides the improvement in the technical design of the solar cells, a better understanding of the defect structure of the material is certainly also required to reach this goal. Solar cell fabricated on polycrystalline material, either bulk or thin films can potentially be cost effective when used in terrestrial photovoltaic conversion systems. The performance of polycrystalline solar cells is usually reduced because of the larger number of recombination centers introduced by the grain boundary states. Since the grain size in the polycrystalline films is in the range 0.1-1 μm, the grain boundaries cannot only introduce a high concentration of electronic states but may also interact strongly with other intrinsic and extrinsic point defects. Therefore, it is evident that an understanding of experimental results in polycrystalline materials has to take into account the defect structure of the grain boundaries. The physical properties of CIS based materials can easily be tailored by proper control of the deposition conditions. The optical band gap of CuInSe$_2$ (~1.02 eV) being less than the optimum value (~ 1.4-1.5 eV) for solar photovoltaic conversion, addition of Ga to the CIS matrix was found to be advantageous due to the fact that it would result in an increase in the band gap, $E_g$, of the absorber material. Thus, an improved device performance may easily be obtained due to the higher open-circuit voltage, $V_{oc}$. Further; improving the absorber quality with reduced grain boundary trap states can also attain a comparatively higher $V_{oc}$. Generally, increase in the grain size reduces losses at the grain boundaries and increases the short-circuit current density. So, for a polycrystalline material like CIS and CIGS, tailoring of the band gap of the absorber layer along with the reduction of barrier height will be important for improved device performance. To achieve this goal, the polycrystalline cell efficiency must increase. A severe limitation to the cell efficiency is due to the grain boundaries and their influence on the carrier recombination. The operation of solar cells under AM1 illumination is an important parameter to study with a view to reduce the cost of photovoltaic power.
generation. The model can be used to determine any of the three parameters: grain size, grain boundary surface recombination velocity and short circuit photocurrent of the CIGS thin-film solar cell. This can also be used to study cell design modifications to improve the efficiency e.g. grain boundary passivation by different processes. It is very well-known that the efficiency of a solar cell strongly depends upon the recombination of minority carriers at the grain boundaries. A reduction in grain size increases the recombination, which reduces the effective diffusion length thereby reducing the short circuit photocurrent.

2 Theory

The purpose of the present study is to investigate the influence of grain size ($d_G$) and the effective surface recombination velocity of the minority carriers ($S_{GB}$) on the short-circuit current density ($J_{SC}$) of the polycrystalline CIGS solar cell. Also, by comparing these theoretical results with the experimental for the variation of ($J_{SC}$) with $d_G$, the grain-boundary recombination velocity for CIGS solar cells have been determined.

For this purpose we consider a semi-infinite polycrystalline semiconductor sample with a Schottky barrier at the top surface $z = 0$. The grain boundaries are considered to be combination planes oriented perpendicular to the junction. Shockley’s filament theory can be used to solve the three-dimensional boundary-value problem and to describe the intra-grain and grain boundary recombination current in the no illuminated cell. When the sample is illuminated, the total short-circuit photocurrent density is given by

$$J_{SC} = J_1 + J_2 \ldots (1)$$

where, $J_1$ is the current due to free minority carriers collected by drift and $J_2$ is the current due to diffusion outside the depletion region $\omega$.

Now, if we consider that the probability $P(z)$ of a photo generated carrier in the depletion region to be collected by the junction and is given by the relation,

$$P(z) = \exp\left( -\frac{z}{L_{drift}} \right) \ldots (2)$$

The current $J_1$ is given by the relation:

$$J_1 = q \cdot g \cdot \int_{0}^{\infty} P(z) dz \ldots (3)$$

where $g$ is the carrier generation rate and $\omega$ is the depletion width.

Substituting Eq. (2) in Eq. (3), we get:

$$J_1 = q \cdot g \cdot \int_{0}^{\infty} \exp\left( -\frac{z}{L_{drift}} \right) dz$$

or,

$$J_1 = L_{drift} \cdot q \cdot g \cdot \left[ 1 - \exp\left( -\frac{\omega}{L_{drift}} \right) \right] \ldots (4)$$

where $L_{drift}$ is given by:

$$L_{drift} = \frac{\mu^* \tau^* V_{bi}}{\omega}$$

such that $\mu^*$ is the effective mobility of the minority carriers; $V_{bi}$ is the diffusion potential of the junction; $\tau^*$ is the effective minority carrier lifetime and can be obtained from Shockley’s filament theory and defined as,

$$\tau^* = \left( \frac{1}{\tau_b} + 2 \cdot D^* \cdot b_0^2 \right)^{-1} \ldots (5)$$

$\tau_b$ is the lifetime of the minority carriers in a single crystal.

$D^*$ is the effective minority carrier diffusion coefficient and can be calculated using:

$$D^* \equiv \left( \frac{K T}{q} \right) \cdot \mu^* \ldots (6)$$

for non-degenerate material.

Value of $b_0$ is obtained from the solution of the transcendental equation:

$$b_0 \cdot \tan\left( b_0 \frac{d_G}{2} \right) = \frac{S_{GB}}{D^*} \ldots (7)$$

$S_{GB}$ is the effective surface recombination velocity of minority carriers at the edge of the grain boundary space charge region. In order to calculate the current $J_2$, first we consider a plane source of strength $G_0$ located outside the depletion region of the barrier and at the depth $\xi$ from the sample surface. In this case the total concentration of excess minority carriers $\Delta n(z)$ in a plane parallel to the semiconductor is given by:

$$\Delta n(z) = G_0 \cdot \exp\left( -\frac{z}{L_{drift}} \right) \ldots (8)$$
\[
\Delta n(z) = \frac{G_0\tau}{2D*} \left\{ \exp\left[\frac{z - \xi}{L*_{\text{dif}}} \right] - \exp\left[\frac{z + \xi}{L*_{\text{dif}}} \right] \right\} \quad \cdots (8)
\]

If \( P(w) \) is the probability of the carrier at the depletion region edge (\( z = \omega \)) to be collected by the junction (\( z = 0 \)), then the diode current \( J_2 \) due to plane source is given by:

\[
J'_2 = qD* \frac{\partial \Delta n(z)}{\partial z} \bigg|_{z=\omega} P(w)
\]

or

\[
J'_2 = qG_0 \exp\left[\frac{-(z - w)}{L*_{\text{dif}}} \right] P(w)
\]

Therefore, for solar illumination the current \( J_2 \) due to the bulk contribution is obtained by integration of above relation with respect to continuous source of carriers.

Thus we get the value of \( J_2 \)

\[
J_2 = qG_0 \exp\left(\frac{\omega}{L*_{\text{dif}}} \right) \int_{\omega}^{\infty} P(\omega) \exp\left(\frac{-z/L*_{\text{dif}}}{} \right) \quad \cdots (9)
\]

Substituting value of \( P(w) \) from Eq. (2) one gets for \( z = \omega \):

\[
J_2 = qG_0 \frac{L*_{\text{dif}}}{L*_{\text{drift}} + L*_{\text{dif}}} \exp\left(\frac{-\omega}{L*_{\text{drift}}} \right) \quad \cdots (10)
\]

where \( L*_{\text{dif}} = (\sqrt{D* \tau_p}) \) is the effective diffusion length in the polycrystal.

It can be verified from the above equations that if the effective diffusion length tends to zero (\( L*_{\text{dif}} \rightarrow 0 \)), then the short-circuit current is due to pure drift collection (\( J_{SC} = J_1 \)), while if \( L*_{\text{dif}} \rightarrow \infty \), the current is due to diffusion collection (\( J_{SC} = J_2 \)).

3 Results and Discussion

In the derivation given above for ease of calculation, a few assumptions have been made viz. (a) The sample is semi-infinite - this assumption can be fulfilled if the thickness of the sample is at least few multiples of the diffusion length. (b) There are no power losses due to reflection and electrode coverage. It has been observed that the reflections and electrode coverage introduce an error of 10-15% for the diode current. So, the theoretical values of \( J_{SC} \) should be reduced by the same factor, but this will not hinder the study of the influence of the grain size and grain boundary recombination velocity on short-circuit current density of the solar cell. The variation of short circuit current density with the grain-boundary recombination velocity for different values of grain size is plotted in Fig. 1. The short-circuit photocurrent density decreases as the grain-boundary recombination velocity increases. In the present calculations, the built-in potential of the junction is taken to be as 0.6 V and the depletion width is assumed to be 2000Å. The mobility for 0.5 μm grain size has been taken to be 8.46 cm²/Vs, whereas for \( d_G=1.0 \) μm it is taken to be 38.2 cm²/Vs. The value of mobility in this range is assumed to vary linearly. The generation rate for AM1 illumination has been taken as \( 10^{21} \) cm⁻³ s⁻¹. Fig. 2 shows the comparison between the

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Fig. 1—Variation of short circuit photocurrent density \( J_{SC} \) with the grain boundary recombination velocity \( S_{GB} \) in a polycrystalline CIGS solar cell under AM1 illumination for different grain sizes (a), (b).

Fig. 2—Variation of short circuit photocurrent density \( J_{SC} \) with the grain size \( d_G \). The continuous lines are the theoretical curves and experimental point represented (•) \( d_G = 0.7 \) and 1.0 μm respectively. (a) \( S_{GB} = 10^3 \) cm/s, (b) \( S_{GB} = 10^4 \) cm/s, (c) \( S_{GB} = 10^5 \) cm/s.
theoretical and the experimental values of short-circuit current density versus with grain size under AM1 illumination\textsuperscript{9,10}. The fit shows that the grain-boundary recombination velocity in CIGS solar cells is about $10^3$ (cm s\textsuperscript{-1}).

4 Conclusion

This model is useful to determine the surface recombination velocity when grain size and current density are known. The present model can be explained for any other inorganic polycrystalline solar cells. With the decrease in surface recombination velocity ($S_{GB}$) and a large increase in $J_{SC}$ for large grain size as compared to small grain size, it may be suggested that for large grain size, the $J_{SC}$ is controlled by surface recombination velocity $S_{GB}$, whereas for small grain size, the grain size plays a dominant role. The fit between the theoretical and experimental results shows that the surface recombination velocity for typical polycrystalline CIGS solar cells is about $10^3$ cm/sec, which is plausible.

References