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# Study of $CdS/Cu(In,Ga)Se_2$ interface by using *n* values extracted analytically from experimental data

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**Abstract**

This paper presents that an analytical method based on Lambert W-function can be applied to estimate the value of the diode ideality factor *n*, of a $ZnO/CdS/Cu(In,Ga)Se_2$ (CIGS) solar cell by using its dark current–voltage characteristics. The method is tested at different temperatures in the dark and found that the resulting $n(T)$ values are in good agreement with those estimated experimentally from the slopes of the straight-line regions of Log $I$–$V$ plots. The suggested values of $n(T)$ under illumination are also determined using the exact explicit analytic solutions for the current–voltage relation expressed in terms of Lambert W-functions and experimentally estimated parasitic series and shunt resistances ($R_s$, $R_{sh}$), diode saturation current ($I_o$), open circuit voltage ($V_{oc}$) and short circuit current ($I_{sc}$) values at various temperatures. Temperature dependence of the diode ideality factor revealed that after illumination still tunnelling enhanced interface recombination mechanism dominates the current transport with relatively low tunnelling energy as compared to the dark case.


*Keywords:* Ideality factor; Lambert W-function; Tunnelling; Solar cell

## 1. Introduction

The forward current density of a typical pn junction device is generally determined by the empirical formula (Sze, 1981),

$$J_F = J_o \exp(AV) \tag{1}$$

where the coefficient $A$ is given as $A = q/nkT$, $n$ is the ideality factor and $J_o$ is the saturation current density defined by

$$J_o \propto \exp\left(\frac{-E_a}{kT}\right) \tag{2}$$

$E_a$ is the activation energy. All these equations indicate that the transport mechanism can be characterised by the temperature dependence of the parameters $A$ and $J_o$. Therefore, the properties of the ideality factor can give some insight into the current transport mechanisms.

If current transport is dominated by any of the thermally activated mechanisms like injection, interface or space charge recombination, the diode ideality factor is independent of temperature and takes values between 1 and 2 depending on the current transport and doping concentrations of the n and p-type layers (Fahrenbruch and Bube, 1983). For example, $n = 1$ when the forward current is limited by thermionic emission. Shockley–Read–Hall (SRH) model assumes that recombination in the space charge region taking place via a single trap level within middle of the gap of low doped side of the junction provides n $\sim 2$ and for an exponential defect distribution, the value of n may lie between 1 and 2. The interface recombination dominated current transport determines that the value of $n$ lies between $2 > n > 1$ and depends on the ratio

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$n = 1 + \varepsilon_p N_A / \varepsilon_n N_D$ where $N_D$ and $N_A$ are the donor and acceptor concentrations and $\varepsilon_n$ and $\varepsilon_p$ are the dielectric constants of n and p-type regions, respectively.

If recombination at p/n junction interface is enhanced by tunnelling $n$ is given by (Padovani and Stratton, 1966),

$$n = \frac{E_{00}}{kT}\coth\left(\frac{E_{00}}{kT}\right) \tag{3}$$

where $E_{00}$ is a characteristic tunnelling energy depending on the doping concentration. For the case of tunnelling enhanced bulk recombination the ideality is described by (Rau et al., 2000)

$$1/n = \frac{1}{2}\left(1 - \frac{E_{00}^2}{3(kT)^2} + \frac{T}{T^*}\right) \tag{4}$$

$kT^*$ is the characteristic energy of the exponential distribution of recombination centers in the bulk of the material. If the contribution of tunnelling is negligible Eq. (4) becomes

$$1/n = \frac{1}{2}\left(1 + \frac{T}{T^*}\right) \tag{5}$$

For tunnelling dominated current transport (Fahrenbruch and Bube, 1983) the slope of the ln $J_F$–$V$ plot A, is essentially temperature independent and the diode ideality factor values are become strongly dependent on temperature and may have values $n(T) \gg 2$.

The value of $n$ can be estimated experimentally directly from the slopes of the straight-line regions of dark Log $I$–$V$ plots where there are no series and shunt resistance effects. However, the dark $I$–$V$ characteristics of solar cells are customarily described by an equivalent circuit model that includes series resistance and shunt conductance. Over the years several methods have been suggested for extracting the value of $n$ from current–voltage data with considerable series and shunt parasitics. Most of these methods are based on illuminated solar cells current–voltage data with a single diode lumped circuit model and are considered the series and shunt resistances (Signal, 1981; Shröder, 1990; Chegaar et al., 2004; Ortiz-Conde et al., 2006; Bouzidi et al., 2007; Bashahu and Nkundabakura, 2007). In addition, an explicit solution for the current and voltage under illuminated condition in terms of Lambert W-function has been proposed to evaluate the value of ideality factor of real solar cell (Jain and Kapoor, 2005).

In this study, the explicit solution for the single diode current equation in terms of W-function is used to extract the value of $n$ at different temperatures from dark current–voltage: temperature ($I$–$V$:$T$) characteristics of a $Cu(In,Ga)Se_2$ solar cell, successfully. The temperature dependent $n(T)$ values are also determined by using the explicit solution for the illuminated current relation in terms of W-function. The $n$–$T$ data is then analysed to suggest the effect of illumination on the previously proposed dark electronic loss mechanism in the solar cell under investigation.

## 2. Experimental

The small area ($0.5\ cm^2$) $Al{:}ZnO/CdS/Cu(In,Ga)Se_2/Mo$/Glass solar cell was prepared in the Institüt für Physikalische Electronic (IPE) at University of Stuttgart. The $Cu(In,Ga)Se_2$ thin layer of about 2 μm was deposited by co-evaporation of Cu, In, Ga and Se onto Mo-coated soda-lime glass substrates. CdS buffer layer of about 0.01 μm thick was deposited by chemical bath deposition and window ZnO layer (≈500 nm) was deposited by RF sputtering technique. The device structure was completed by the evaporation of Al metal grid onto ZnO layer. Details of the fabrication steps are described elsewhere (Stolt et al., 1995). The carrier concentrations of n and p regions of the solar cell under investigation are in the order of $10^{16}\ cm^{-3}$ and $10^{18}\ cm^{-3}$, respectively, so that the device structure can readily be represented as $n^+p$. The efficiency of the investigated device is about 12%.

The temperature dependent $I$–$V$ data were measured in an evacuated closed-cycle helium cryostat (Oxford) heated in the temperature range of 100–300 K by using a Keithley 236 source meter.

## 3. Theory and calculations

The dark forward current of a p–n junction device which modelled by a single exponential expression, with a parasitic series $R_s$, and shunt $R_{sh}$ resistances can be expressed by

$$I = \frac{V - IR_s}{R_{sh}} + I_0\left(\exp\left(\frac{q(V - IR_s)}{nkT}\right) - 1\right) \tag{6}$$

where $I_o$ is the saturation current and $k$ is Boltzmann's constant. The explicit solution for the current in terms of Lambert W-function is (Ortiz-Conde et al., 2006)

$$I = n\frac{kT}{qR_s}\,\text{Lambert W}\left[\frac{qR_sR_{sh}I_0}{nkT(R_s + R_{sh})}\exp\left(\frac{qR_{sh}(V + I_0R_s)}{nkT(R_s + R_{sh})}\right)\right] + \frac{V - I_0R_{sh}}{R_s + R_{sh}} \tag{7}$$

When the experimentally determined values of $I_o$, $R_s$, $R_{sh}$ and $V$ for a given temperature in the dark are inserted to Eq. (7), then an equation in the form of $I(n)$ can be determined.

Since the conduction mechanism in the $n\text{-}ZnO/n\text{-}CdS/p\text{-}Cu(In,Ga)Se_2$ solar cell was previously investigated by dividing the dark Log $I$–$V$ characteristics into two distinct regions (region I: $0.6\ V > V > 0.2\ V$ and region II: $0.8\ V > V > 0.6\ V$ (Bayhan and Kavasoğlu, 2005), $I$ vs. $n$ data is calculated separately for these regions. Temperature dependent $I_o$, $R_s$ and $R_{sh}$ values in region I and II are estimated from current–voltage and impedance measurements, respectively and given in Table 1. The parameter $V$ in Eq. (7) can be any value on the linearly varying part of the Log $I$ vs. $V$ plot for a given temperature and region, see Fig. 1. For example, at 100 K the value of $V$ is chose as 0.4 V for region I and 0.7 V for region II, then $I$ is determined as a function of $n$ in terms of W-function as

Table 1
Some dark and illuminated parameters of a n-ZnO/n-CdS/p-Cu(In,Ga)$Se_2$ solar cell determined at various temperatures

| Temperature (K) | | 100 | 140 | 200 | 240 | 300 |
|---|---|---|---|---|---|---|
| $V_{oc}$ (V) | | 0.750 | 0.720 | 0.690 | 0.664 | 0.610 |
| $I_{ph}$ (A) | | 0.0140 | 0.0138 | 0.0135 | 0.0133 | 0.0130 |
| $R_{sh}$ (Ω) | | $82 \times 10^4$ | $68 \times 10^4$ | $48 \times 10^4$ | $34 \times 10^4$ | $23 \times 10^4$ |
| $R_s$ (Ω) | | 8.0 | 8.6 | 9.0 | 9.5 | 10.0 |
| $I$ (A) (dark) | Region I (at 0.4 V) | $6.50 \times 10^{-6}$ | $8.10 \times 10^{-6}$ | $9.85 \times 10^{-6}$ | $1.42 \times 10^{-5}$ | $4.60 \times 10^{-3}$ |
| | Region II (at 0.7 V) | $8.10 \times 10^{-5}$ | $9.90 \times 10^{-4}$ | $1.28 \times 10^{-4}$ | $2.07 \times 10^{-4}$ | $1.20 \times 10^{-3}$ |
| $I_o$ (A)(dark) | Region I | $2.00 \times 10^{-7}$ | $3.95 \times 10^{-7}$ | $4.35 \times 10^{-7}$ | $6.00 \times 10^{-7}$ | $1.05 \times 10^{-6}$ |
| | Region II | $4.70 \times 10^{-8}$ | $1.05 \times 10^{-7}$ | $1.50 \times 10^{-7}$ | $1.90 \times 10^{-7}$ | $4.50 \times 10^{-7}$ |

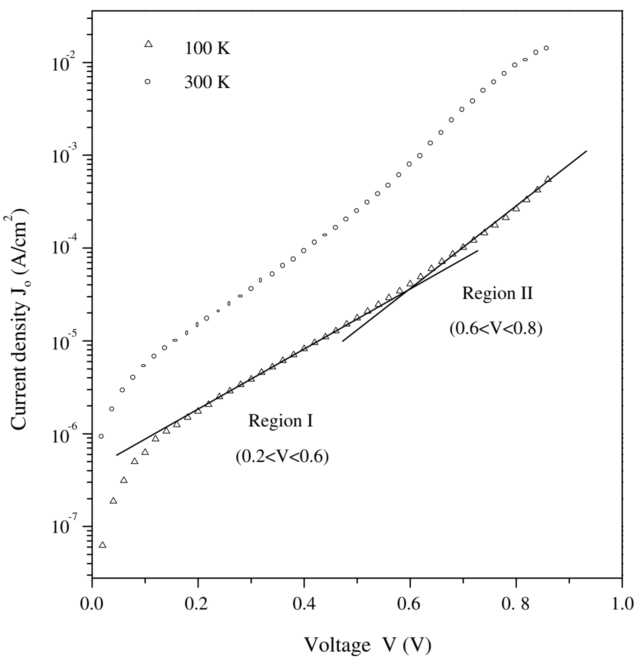


Fig. 1. The dark $I$–$V$ characteristics of a n-ZnO/n-CdS/p-Cu(In,Ga)$Se_2$ solar cell at 100 K and 300 K.

$$I_{\text{regionI}} = n \times 1.08 \times 10^{-3} \text{ Lambert W} \times \left[\frac{1.85 \times 10^4}{n} \exp\left(\frac{46.37}{n}\right)\right] + 2.88 \times 10^{-7} \tag{8a}$$

$$I_{\text{regionII}} = n \times 1.08 \times 10^{-3} \text{ Lambert W} \times \left[\frac{4.36 \times 10^5}{n} \exp\left(\frac{81.16}{n}\right)\right] + 8.07 \times 10^{-7} \tag{8b}$$

By varying the value of $n$ from 1 to 20 regularly, the corresponding value of $I$ is calculated. Typical plots for obtained at 100 K in the dark are illustrated in Fig. 2 Since $I$ $(0.4\text{ V}) = 6.50 \times 10^{-6}$ A in region I and $I$ $(0.7\text{ V}) = 8.10 \times 10^{-5}$ A in region II, (see Fig. 1.), the corresponding values for the ideality factor on Fig. 2 are found as 13.71 and 10.90, respectively. The $n$ values are estimated at different temperatures with the same procedure and found that these extracted values are in well accordance with those calculated from the slopes of the straight-line regions of Log $I$ vs. $V$ plots (Bayhan and Kavasoğlu, 2005), see Table 2. The confidence intervals of the fits are found as about 0.999.

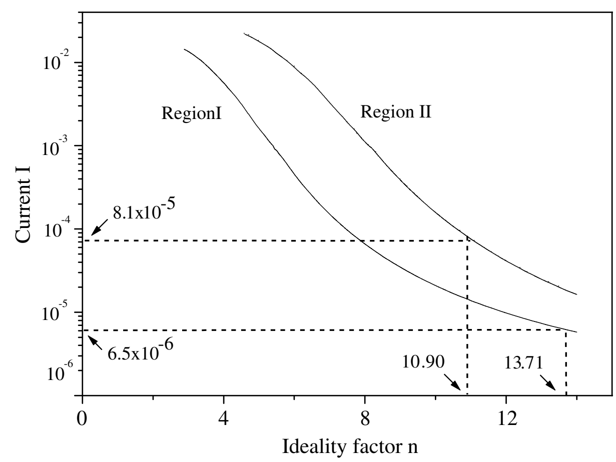


Fig. 2. The dark $I$- $n$ characteristics of a n-ZnO/n-CdS/p-Cu(In,Ga)$Se_2$ solar cell at 100 K.

Under illumination, the current–voltage relation for the single diode model in terms of W-function given by (Jain and Kapoor, 2005) is used

$$I = -n\frac{kT}{qR_s} \text{ Lambert W} \times \left[\frac{qR_sR_{sh}I_0}{nkT(R_s + R_{sh})} \exp\left(\frac{qR_{sh}(V_{oc} + I_0R_s + R_sIph)}{nkT(R_s + R_{sh})}\right)\right] - \frac{V_{oc}}{R_s + R_{sh}} + \frac{R_{sh}(I_0 + I_{ph})}{R_s + R_{sh}} \tag{9}$$

Experimentally estimated $R_s$, $R_{sh}$, $I_o$, open circuit $V_{oc}$ and short circuit $I_{sc}$ current values (see Table 1) are used to obtain $I$–$n$ relation at different temperatures in terms of $W$-function. The typical equations expressed for region I and II at 100 K are

$$I_{\text{regionI}} = -9.15 \times 10^{-7} - n \times 1.08 \times 10^{-3} \text{ Lambert W} \times \left[\frac{1.85 \times 10^{-4}}{n} \exp\left(\frac{99.94}{n}\right)\right] + 0.014$$
$$I_{\text{regionII}} = -9.15 \times 10^{-7} - n \times 1.08 \times 10^{-3} \text{ Lambert W} \times \left[\frac{4.36 \times 10^{-5}}{n} \exp\left(\frac{99.94}{n}\right)\right] + 0.014 \tag{10}$$

During calculations, it is assumed that parasitic resistance values ($R_s$ and $R_{sh}$) are not vary considerably under illumination. Fig. 3 shows the ideality factor vs. current

Table 2
Ideality factors obtained from W-function method and the slope of the Log $I$–$V$ plot under dark condition

| | Temperature (K) | | 100 | 140 | 200 | 240 | 300 |
|---|---|---|---|---|---|---|---|
| n | Experimental (Bayhan and Kavasoğlu, 2005) | Region I | 13.79 | 10.80 | 7.33 | 5.99 | 4.06 |
| | | Region II | 11.69 | 8.47 | 5.94 | 4.82 | 3.46 |
| | Lambert W-function method | Region I | 13.71 | 11.04 | 7.53 | 6.01 | 4.08 |
| | | Region II | 10.90 | 8.46 | 5.95 | 4.82 | 3.44 |

characteristics for both regions at 100 K. Theoretically, one can obtain the value of $n$ as a function of temperature by substituting values of series and shunt parasitics, $V = V_{oc}$, $I_{ph} = I_{sc}$ and $I = 0$ into the current–voltage–temperature relationship $I = I_{ph} - \frac{V+IR_s}{R_{sh}} - I_o(\exp\frac{q(V+IR_s)}{nkT} - 1)$. Thus, the expected value of $n$ can be estimated from Fig. 3 by considering the value of $x$-axis at which $I$ is zero. The variation given in Fig. 4 shows the temperature dependence of the ideality factor extracted by Lambert W-function method under illumination. This graph is also contains the $n$–$T$ data of the dark case in comparison.

In the previous work, the electrical conduction in n-CdS/p-Cu(In,Ga)$Se_2$ device was suggested to be dominated by tunnelling enhanced interface recombination mechanism the dark (Bayhan and Kavasoğlu, 2005). The presence of this unexpected route was attributed to the presence of Cu-rich p-$CuGaSe_2$ layer on the absorber p-Cu(In,Ga)$Se_2$ surface. The proposed model predicts that tunnelling of holes from the bulk of the Cu(In,Ga)$Se_2$ layer into the interface states at n-CdS/p-$CuGaSe_2$ interface and subsequent recombination with electrons available in the buffer CdS layer yields the temperature dependence of the diode ideality factor as given by Eq. (3). The tunnelling energies in the dark were calculated as $E_{00} = 69$ meV and 103.5 meV for regions I and II, respectively.

Since variations plotted in Fig. 4 indicate that $n$ (T) » 1, the contribution of tunnelling could still be important under illumination. The extracted $n$–$T$ data is found to fit very well on the theoretical expression given by Eq. (3) and from these fits the tunnelling energies of the illuminated case are calculated as about 60 and 66 meV for

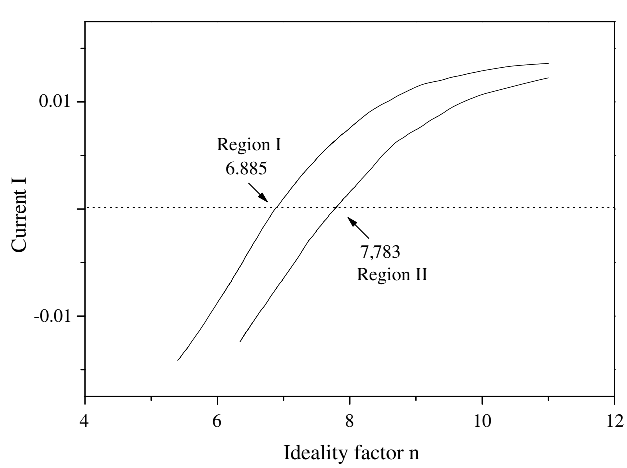


Fig. 3. The illuminated $I$ - characteristics of a n-ZnO/n-CdS/p-Cu(In,Ga)$Se_2$ solar cell at 100 K.

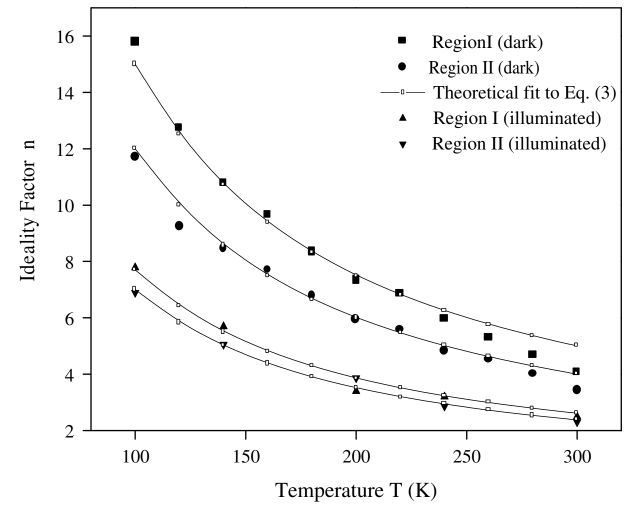


Fig. 4. The temperature dependence of the ideality factor obtained from W-function method both for under dark and illuminated conditions.

regions I and II, respectively. Although a detailed analysis of the current transport mechanism needs the evaluation of the temperature dependence of the $I$–$V$ data, lower $E_{00}$ values can be ascribed to the reduction of the tunnelling contribution under illumination (Rau et al., 2000). It is well known that, illumination might result in a metastable increase of the emission rate of interface trap states and induce the band bending by decreasing the distance between the Fermi level and the bottom of the conduction band (Nadenau et al., 2000). A shallow acceptor level with an activation energy around 50 meV has previously been detected in the solar cell under investigation and the presence of this trap was proposed to be correlated to the appearance of Cu-rich $CuGaSe_2$ layer formed on the Cu(Ga,In)$Se_2$ absorber (Bayhan and Kavasoğlu, 2006). The present understanding is that the shallow acceptor level with an activation energy at about 50 meV, might be the involved in the capture of photo generated holes and the reduction of the negative charge in the space charge layer which shifts the Fermi level towards the conduction band and lowers the tunnelling barrier for electrons emitted from interface states.

## 4. Conclusion

A simple method based on Lambert W-function is shown to be applicable for the determination of the temperature dependent diode ideality factor values in the dark. The method is successfully applied to an efficient n-ZnO/n-

CdS/p-Cu(In,Ga)$Se_2$ solar cell and the results obtained are in good agreement with those published previously.

The electronic loss mechanism under illumination is investigated using diode ideality factor values obtained by Lambert W-function method at different temperatures in between 100 K and 300 K. In these calculations it is assumed that parasitic effects do not vary much under illumination. The temperature dependence of the extracted $n$ values has been shown to be in good agreement with the theoretical expression given for tunnelling enhanced interface recombination mechanism. The reduction of tunnelling energy might possibly be attributed to the effect of illumination on the interface trap states and thus to the decrease of the distance between the Fermi level and the bottom of the conduction band. An acceptor level at about 50 meV which is identified in this solar cell by admittance measurements in the previous work, can be correlated for the reduction of the negative charge in the space charge layer and thus lowering the tunnelling barrier for electrons emitted from interface states.

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