Estimation of the local ideality factor of CdS/Cu(In,Ga)Se₂ Interface from experimental data

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Abstract
This article suggests a simple method to calculate the local ideality factor n for a ZnO/CdS/Cu(In,Ga)Se₂ solar cell from the I-V:T data in dark. An empirical model is incorporated into the single-diode model in order to remove its implicit nature and to ease calculations. The forward current-voltage characteristics have been analyzed on the basis of standard thermionic emission (TE) theory and the extracted values of n at different temperatures from dark I–V:T characteristics of a CdS/p-Cu(In,Ga)Se₂ solar cell reveals that the conduction is dominated by tunneling enhanced interface recombination mechanism. The tunneling energies $E_{00}$ are calculated from the fit at three voltage values 0.4 V, 0.6 V, and 0.8 V and found to be about 87.6, 94.8, and 95.3 meV, respectively. The influence of the temperature on the local ideality factor n has been analyzed and found that the ideality factor decreases exponentially when the temperature increases.

Keywords: Solar cell, Ideality factor, Schottky contact, thermionic emission.

1. Introduction
In an ideal Schottky diode, the flow of current is solely due to thermionic emission TE mechanism and the ideality factor n should be equal to unity. However, due to various factors such as device temperature, dopant concentration, density of interface states, device area, structural properties of interface etc., the current-voltage characteristics of Schottky contact exhibit deviations from ideal case with temperature dependent ideality factor [1,2]. Generally, the ideality factor increases with decrease in
temperature. This phenomenon is commonly referred as “T₀-effect” and was first proposed by [3]. The barrier height of such device is found to decrease with the fall in operating temperature.

The knowledge of the ideality factor \( n \) is of vital importance in identifying the current transport mechanisms and interfacial properties of a pn-junction device. Accurate evaluation of the ideality factor versus temperature, in particular, can give valuable information about the main recombination routs in the devices [4]. Values of the ideality factor \( n \) could be estimated from the \( I-V \) characteristics by calculating the slopes of the straight line segments of dark log \( I \) vs. \( V \), ignoring the effects of shunt and series resistances. However, the dark \( I-V \) characteristics are usually described by an equivalent circuit model that includes shunt and series resistances [5].

Several methods for extracting the value of \( n \) from the \( I-V \) characteristics considering the shunt and series resistances have been suggested during the last two decades. Some of these methods rely on illuminated \( I-V \) data and the subsequently calculated conductance of the device [6-11]. Other methods based on numerical analysis [12,13] and on the Co-content function [14] from the exact explicit analytical solutions of the \( I-V \) data are reported.

Later, Jain and Kapoor [15] have introduced a simple analytical method based on the Lambert W-function. In their method, they have calculated the junction ideality factor of a solar cell directly from the \( I-n \) curve using Lambert W-function. Recently, Bayhan and Kavasoglu [16] have presented an analytical method for extracting the ideality factor \( n \) of a pn-junction device based on the Lambert W-function and the dark \( I-V \) data.

In this article a simple method based on incorporating an empirical model into the single diode current equation is used successfully to determine the local ideality factor \( n \). An explicit solution of the resulting equation is used to extract the value of \( n \) at different temperatures from dark current–voltage: temperature (\( I-V:T \)) characteristics of a ZnO:Cu(In,Ga)Se₂ solar cell. The \( I-V:T \) data are extracted from ref. [17].

2. Theory and calculations

In general, the forward current density of a typical pn-junction device can be determined by the following empirical formula [18],

\[
J_F = J_0 \exp(AV) \quad 1
\]

where the parameter \( A \) is equal to \( q/\eta nkT \). The ideality factor \( n \) is introduced to describe the deviation of the experimental \( I-V \) data from the ideal thermionic emission diffusion, \( q \) is the electronic charge \( 1.6 \times 10^{-19} \text{C} \), \( k \) is the Boltzmann’s constant \( 1.38 \times 10^{-23} \text{J/K} \), \( T \) is the temperature in Kelvin, and \( J_0 \) is the saturation current density defined by

\[
J_0 \propto \exp \left( \frac{-E_a}{kT} \right), \quad 2
\]

\( E_a \) is the activation energy. These equations indicate that the transport mechanism can be characterized by the temperature dependence of the parameters \( A \) and \( J_0 \). Therefore, the ideality factor can give some insight into the current transport mechanisms.

If the current transport is dominated by any of the thermally activated mechanisms such as injection, interface or space charge recombination, the diode ideality factor \( n \) is independent of temperature with values ranging between 1 and 2 depending on the current transport and doping concentrations of the n and p-type layers [19]. For example, when the forward current is limited by thermionic emission \( n \) is equal to 1. Shockley–Read–Hall (SRH) model assumes that the recombination in the space charge region is taking place via a single trap level located near the middle of the gap of low doped side of the junction gives \( n \sim 2 \), and for an exponential defect distribution, the value of \( n \) may have values between 1 and 2. On the other hand, when current transport is dominated by interface recombination the value of \( n \) lies between \( 2 > n > 1 \).
and is dependent on the ratio \( n = 1 + \varepsilon_p N_A / \varepsilon_n N_D \) 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 materials, respectively.

If recombination at the interface of the pn-junction is enhanced by tunneling \( n \) is described by [20],

\[
n = \frac{E_{00}}{kT} \coth \left( \frac{E_{00}}{kT} \right),
\]

\( E_{00} \) is a characteristic tunneling energy measuring the amount of tunneling contribution to the recombination process. For the tunneling enhanced bulk recombination case, the ideality factor is given by the following equation [21]

\[
\frac{1}{n} = \frac{1}{2} \left( 1 - \frac{E_{00}^2}{3(kT)^2} + \frac{T}{T^*} \right),
\]

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

\[
\frac{1}{n} = \frac{1}{2} \left( 1 + \frac{T}{T^*} \right).\]

For tunneling dominated transport [19], the slope \( A \) of the \( \ln J_F - V \) graph is essentially temperature independent, and the values of the diode ideality factor are become strongly dependent on temperature and may have values \( n(T) \gg 2 \).

In the single-diode model a current source is used to model the incident solar irradiance, a diode for the polarization phenomena, a series resistance and a parallel resistance to account for the power losses. Using Kirchhoff’s law, the cell terminal current is

\[
I = I_{ph} - I_0 \left[ \exp \left( \frac{V + I_R s}{V_c n} \right) - 1 \right] - \frac{V + I_R s}{R_{sh}},
\]

where \( I_{ph} \) and \( I_0 \) are the photo-generated current and the dark saturation current of the PV system, respectively, and \( V_L = N_k kT/q \) is the thermal voltage of the PV system with \( N_k \) cells connected in series, \( R_s \) and \( R_{sh} \) are the cell series resistance and the cell shunt resistance, respectively. One can modify Eq. (6) in order to express the dark forward current of a pn-junction device as

\[
I = \frac{V - IR_s}{R_{sh}} + I_0 \left[ \exp \left( \frac{V - I_R s}{V_c n} \right) - 1 \right].
\]

Equation (7) describes the single-diode model. It is an implicit function, i.e. have the form \( I = f(V, I) \). Such implicit nature of the model makes the method for adjusting the model parameters more difficult.

Some other models that can generate the IV curves from the manufacturer’s datasheet of a PV system have been suggested. Among these models is the model that can be expressed as [22]:

\[
I_{TA} = I_{sc} - C_1 \exp \left( - \frac{V_{oc}}{C_2} \right) \left[ \exp \left( \frac{V}{C_2} \right) - 1 \right],
\]

where the \( I_{sc} \) and \( V_{oc} \) are the short circuit current and the open circuit voltage, respectively. The coefficients of the model equation \( C_1 \) and \( C_2 \) can be obtained either graphically or analytically. In this work Eq. (8) is modified to account for the dark situation by having the following form

\[
I_{TA} = C_1 \exp \left( - \frac{V_{max}}{C_2} \right) \left[ \exp \left( \frac{V}{C_2} \right) - 1 \right].
\]

In order to find the coefficients \( C_1 \) and \( C_2 \) one needs two equations. Thus two points from the experimental data are needed to be specified in order to obtain \( C_1 \) and \( C_2 \). One can chose the point of maximum voltage and current (\( V_{max} \) and \( I_{max} \)) from the experimental data. Another point (an optional point \( V_{opt} \) and \( I_{opt} \)) is chosen at 0.66 V. Thus substituting these two points into Eq. 9 one obtains the following equations

\[
I_{max} = C_1 \exp \left( - \frac{V_{max}}{C_2} \right) \left[ \exp \left( \frac{V_{max}}{C_2} \right) - 1 \right],
\]

\[
I_{opt} = C_1 \exp \left( - \frac{V_{opt}}{C_2} \right) \left[ \exp \left( \frac{V_{opt}}{C_2} \right) - 1 \right].
\]

One can solve Eq. (10) and Eq. (11) either graphically or simultaneously in order to obtain values of \( C_1 \) and \( C_2 \). Figure 1 shows a graphical solution of \( C_1 \) and \( C_2 \).
Incorporating the obtained values of $C_1$ and $C_2$ into Eq. (9) one is able to generate the dark $IV$ characteristics of a pn-junction. Figure 2 shows the good match between the experimental and modeled dark $IV$ data.

To ease the calculations, the implicit nature of Eq. (7) can be removed by incorporating Eq. (9) into Eq. (7) to get

$$I = \frac{V - I_{TA}R_s}{R_{sh}} + I_0 \left\{ \exp \left[ \frac{(V - I_{TA}R_s)}{V_T} \right] - 1 \right\}. \quad 12$$

One can solve the last equation to obtain the following expression of the local diode ideality factor $n(I)$

$$n(I) = \left( \frac{q}{kT} \right) \left\{ \frac{V - I_{TA}R_s}{\ln \left[ I_{sh} + I_0 \right] - \ln I_0} \right\}. \quad 13$$

Substituting the experimental values of current and voltage in the last equation one can obtain the local ideality factor $n$ at each $I-V$ experimental data point. Some values of the dark parameters of a n-Zn-CdS/p-Gu(In,Ga)Se$_2$ solar cell used to calculate the local ideality factor at various temperatures are shown in table 1.
Table 1. Some dark parameters of a n-Zn-CdS/p-Gu(In,Ga)Se$_2$ solar cell used to calculate the local ideality factor at various temperatures [17].

<table>
<thead>
<tr>
<th>Temperature(K)</th>
<th>$R_{sh}$ (Ω) x $10^4$</th>
<th>$R_s$ (Ω)</th>
<th>$I_0$ x $10^{-7}$ (A)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>82</td>
<td>8.0</td>
<td>0.470</td>
</tr>
<tr>
<td>140</td>
<td>68</td>
<td>8.6</td>
<td>1.05</td>
</tr>
<tr>
<td>200</td>
<td>48</td>
<td>9.0</td>
<td>1.50</td>
</tr>
<tr>
<td>240</td>
<td>34</td>
<td>9.5</td>
<td>1.90</td>
</tr>
<tr>
<td>300</td>
<td>23</td>
<td>10.0</td>
<td>4.50</td>
</tr>
</tbody>
</table>

3. Results and discussion:

Deviations of the ideality factor from one indicate that there are unusual recombination mechanisms taking place, or that the recombination is changing in magnitude. This makes the ideality factor a powerful tool for examining the recombination in a device. The local ideality factor $n$ of the device in dark can be calculated using Eq. (13) at each point of the experimental data and using the parameters in Table 1. The variation of the local ideality factor $n$ with log $I$ at various temperatures is shown in Fig. 3. It is clear from the figure that at each temperature there are three, almost, linear regions with different slopes. At relatively low current $n$ increases with increasing log $I$ in the first region. The local ideality factor continues increasing in the second region but with smaller slope. In region three the values of $n$ start to decrease with increasing log $I$. It is believed that they correspond to three different regimes. Also, it is clear that the local ideality factor $n$ increases with decreasing temperature.

![Figure 3](image_url)  

Fig. 3 The variations of the local ideality factor as a function of current at various temperature values.
Figure 4 illustrates the variations of the local ideality factor $n$ obtained from Eq. (13) with voltage at various temperatures. At low applied voltage $n$ increases with increasing $V$. The values of $n$ start dropping at higher voltages. Also, it is clear that the local ideality factor $n$ increases with decreasing temperature.

![Graph showing variations of local ideality factor](image)

$E_{00}^0 = 87.6$ meV at 0.4 V
$E_{00}^0 = 94.8$ meV at 0.6 V
$E_{00}^0 = 95.3$ meV at 0.8 V

Figure 5 represents the dependence of the local ideality factor $n$ on temperature at three different voltages. Since the variations plotted in figure indicate that $n$ ($T$) $\gg$ 1, the contribution of tunneling could be important. The extracted $n$–$T$ data is found to fit well on the theoretical expression given by Eq. (3) for the case when the current through Schottky junction is dominated by thermionic field emission and from these fits the tunneling energies $E_{00}^0$ are calculated at three voltage values 0.4 V, 0.6 V, and 0.8 V and found to be about 87.6, 94.8, and 95.3 meV, respectively. Bayhan and Kavasoglu [23] have suggested that the electrical conduction in CdS/p-Cu(In,Ga)Se$_2$ device to be dominated by tunneling enhanced interface recombination.

![Graph showing variation of local ideality factor with temperature](image)
mechanism in the dark. The presence of this unexpected route was attributed to the presence of Cu-rich p-CuGaSe\textsubscript{2} layer on the absorber p-Cu(In,Ga)Se\textsubscript{2} surface. The proposed method predicts that tunneling of holes from the bulk of the Cu(In,Ga)Se\textsubscript{2} layer into the interface states at n-CdS/p-CuGaSe\textsubscript{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).

To express the robustness of the method one can substitute the obtained values of theoretical local diode ideality factor $n$ into Eq. (12) and plot the IV characteristics as shown in Fig.6.

![Figure 6. I-V characteristics at various temperatures. Points are experimental data. Line is calculated data.](image)

4. Conclusions

A simple method based on incorporating an empirical model into the single diode current equation is applied to determine the local ideality factor $n$. The extracted values of $n$ at different temperatures from dark $I$–$V$: $T$ characteristics of a CdS/p-Cu(In,Ga)Se\textsubscript{2} solar cell reveals that the conduction dominated by tunneling enhanced interface recombination mechanism. The tunneling energies $E_{00}$ are calculated from the fit at three voltage values 0.4 V, 0.6 V, and 0.8 V and found to be about 87.6, 94.8, and 95.3 meV, respectively. The local ideality factor $n$ is found to increase with decreasing temperature.

References