Supplementary Information (SI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2024

Supporting Information

Numerical evaluation of bi-facial ZnO/MoTe$_2$ photovoltaic solar cells with N-doped Cu$_2$O as BSF layer focuses on enhancing V$_{OC}$ via device simulation

Arifuzzaman Rajib[1]*, Tapos Chandra Saha,[1] Md. Mustafizur Rahman,[1] Hridoy Sarker,[1]
Ruddro Dhali,[1] Md. Sabbir Hossain Sumon,[1] and Atowar Rahman,[2*]

[1]Department of Electrical and Electronic Engineering, Bangabandhu Sheikh Mujibur Rahman Science and Technology University, Gopalganj-8100, Bangladesh
[2]Department of Electrical and Electronic Engineering, University of Rajshahi, Rajshahi-6205, Bangladesh

[1*]Electronic mail: rajib.apee.38@gmail.com, rajib.eee@bsmrstu.edu.bd
[2*] Email: atowar@ru.ac.bd

S1

Recombination analysis of n-ZnO/p-MoTe$_2$-based PVSC with and without p$^+$-N:Cu$_2$O-BSF layer

Defect assisted recombination called Shockley-read-Hall (SRH) recombination is the most dominant recombination process among the various recombination process in solar cells which able to deteriorate the cell performance mostly. SRH recombination statistics as well as analytical approximation can be performed to understand the qualitative and quantitative extraction of recombination rates at cell regions of the devices such as at the ETL/absorber interface ($R^{i,f}$), in the depletion region (R^d), in the bulk region zone (R^b), and at the BSF layer/absorber interface ($R^{i,b}$).[1] However, the bias voltage (V) and the temperature dependent recombination rates can be expressed as follows:[1]

$$R^{i,f} = R_0^{i,f} e^{\frac{qV}{K_B T}} \tag{1}$$

$$R^{d} = R_0^{d} e^{\frac{qV}{2K_B T}} \tag{2}$$

$$R^{b} = R_0^{b} e^{\frac{qV}{K_B T}} \tag{3}$$

$$R^{i,b} = R_0^{i,b} e^{\frac{qV}{K_B T}} \tag{4}$$

Where K$_B$ defines the Boltzmann constant and $R_0^{i,f}$, R_0^d,R_0^b, and $R_0^{i,b}$ represent the recombination coefficient at the ETL/absorber interface, in the depletion region, in the bulk region zone, and at the BSF layer/absorber interface with zero bias voltage (V=0), in that order. These coefficients ($R_0^{i,f}$, R_0^d,R_0^b, and $R_0^{i,b}$) are essential for the intrinsic properties of material or devices and show effectiveness of the corresponding recombination pathways. The mathematical formula for recombination coefficients ($R_0^{i,f}$, R_0^d,R_0^b, and $R_0^{i,b}$) are expressed as follows:[1]

$$R_0^{i,f} = S_h^f N_V e^{\frac{q\varphi_{b0}}{K_B T}} \tag{5}$$

$$R_0^d = \frac{W_d}{\tau_e + \tau_h} n_i \tag{6}$$

$$R_0^b = \frac{W n_i^2}{\tau_e N_A} \tag{7}$$

$$R_0^{i,b} = S_e^b N_C e^{\frac{E_g - \varepsilon_b}{K_B T}} \tag{8}$$

where S_h^f/S_e^b represent the surface recombination velocity of hole/electron at front/back interface, φ_{b0} is the potential barrier for majority carrier at the interface, q ascribes the electric charge, W_d defines depletion width, τ_e/τ_h are the minority carrier lifetime for electron/hole in the quasi-neutral region, W is the absorber thickness, N_A defines the acceptor density, N_C/N_V describe the effective conduction/valance band density, E_g is the band gap of absorber layer, ε_b is the bulk Fermi-energy separation from the valence band edge.

Now, focusing on the open circuit voltage V_{OC}, assuming that total generation across the absorber layer GaW (W=width of the absorber layer) is equal to the total recombination ($\sum R = R^{i,f} + R^d + R^b + R^{i,b}$), which expressed as:

$$(R_0^{i,f} + R_0^b + R_0^{i,b})\, e^{\frac{qV_{OC}}{K_B T}} + R_0^d e^{\frac{qV_{OC}}{2K_B T}} = G_a W \tag{9}$$

Now solving the Eqn (9) and the V_{OC} can be expressed as follow:

$$V_{OC} = \frac{2K_B T}{q} ln[K_1(\sqrt{G_a K_2 + 1} - 1)] \tag{10}$$

Where,

$$K_1 = \frac{1 \quad R_0^d}{2R_0^{i,f} + R_0^b + R_0^{i,b}} \tag{11}$$

$$K_2 = \frac{4W(R_0^{i,f} + R_0^b + R_0^{i,b})}{(R_0^d)^2} \qquad (12)$$

Using Eqn. (11) and Eqn. (12), the recombination coefficient in the SCR zone is

$$R_0^d = \frac{2W}{K_1 K_2} \qquad (13)$$

It is clearly observed that the recombination coefficient in the SCR zone R_0^d, can be calculated by extracting the values of K_1 and K_2 from the intensity dependent V_{OC} analysis under the white light irradiation condition.

The intensity dependent V_{OC} analysis under monochromatic short and long wavelength are carried out to extract the recombination coefficient at absorber/BSF interface ($R_0^{i,b}$), and surface recombination velocity of electrons at absorber/BSF interface (S_e^b). As the photons energy of SW light source (blue) is well above the band gap of the absorber material, electron and hole pairs are generated near the surface region resulting the most of the SRH recombination is taken place in the vicinity of the front interface (ZnO/$MoTe_2$ interface), which make the recombination at the back interface is approximately zero ($R_0^{i,b} \sim 0$). Therefore, under monochromatic SW light illumination, the coefficient of K_1 and K_2 can be written as:

$$K_1^{SW} = \frac{1 \quad R_0^d}{2R_0^{i,f} + R_0^b} \qquad (14)$$

$$K_2^{SW} = \frac{4W(R_0^{i,f} + R_0^b)}{(R_0^d)^2} \qquad (15)$$

On the other side, the photons energy of LW light source (Red) is nearly equal to the band gap of the absorber, makes nearly uniform generation profile across the absorber layer and the coefficient of K_1 and K_2 can be expressed as:

$$K_1^{LW} = \frac{1 \quad R_0^d}{2R_0^{i,f} + R_0^b + R_0^{i,b}} \qquad (16)$$

$$K_2^{LW} = \frac{4W(R_0^{i,f} + R_0^b + R_0^{i,b})}{(R_0^d)^2} \tag{17}$$

After simplification of Eqn. (14) and Eqn. 16), the recombination coefficient at the back interface can be obtained as:

$$R_0^{i,b} = \frac{1}{2}[\frac{1}{K_1^{SW}} - \frac{1}{K_1^{LW}}] \times R_0^d \tag{18}$$

Now putting the value the recombination coefficient in the SCR zone (R_0^d) have already obtained from Eqn. (13) in Eqn. (18) and we can get the value of the recombination coefficient at the back interface ($R_0^{i,b}$). After that, the recombination rate in the depletion zone and absorber/BSF interface can be obtained utilizing Eqn. (2) and Eqn. (4), respectively from the known values of R_0^d and $R_0^{i,b}$. Finally, the surface recombination velocity of electrons at the back interface (S_e^b) can be extracted by using Eqn. (8) from the known values of $R_0^{i,b}$, N_C, and $E_g - \varepsilon_b$.

In this study, the two different monochromatic wavelengths (450 nm and 800 nm) are carried out to illuminate the designed PVSCs aiming to extract qualitative and quantitative information about the recombination at the back interface with and without N:Cu_2O-BSF layer. **Fig. 1** shows the light intensity (Ga) dependent V_{OC} graphs for without **(b)** and with **(b)** N:Cu_2O-BSF layer. The value of the coefficients K_1 and K_2 are extracted from the fitting of the intensity dependent V_{OC} curves of the **Fig. 1** by using **Eqn. (10), Eqn. (11), and Eqn. (12),** and other recombination coefficients R_0^d, $R_0^{i,b}$, R^d, and **$R^{i,b}$ from** K_1 and K_2 and the surface recombination velocity of electrons at the back interface (S_e^b) from the extracted recombination coefficient are assembled in **Table 1.**

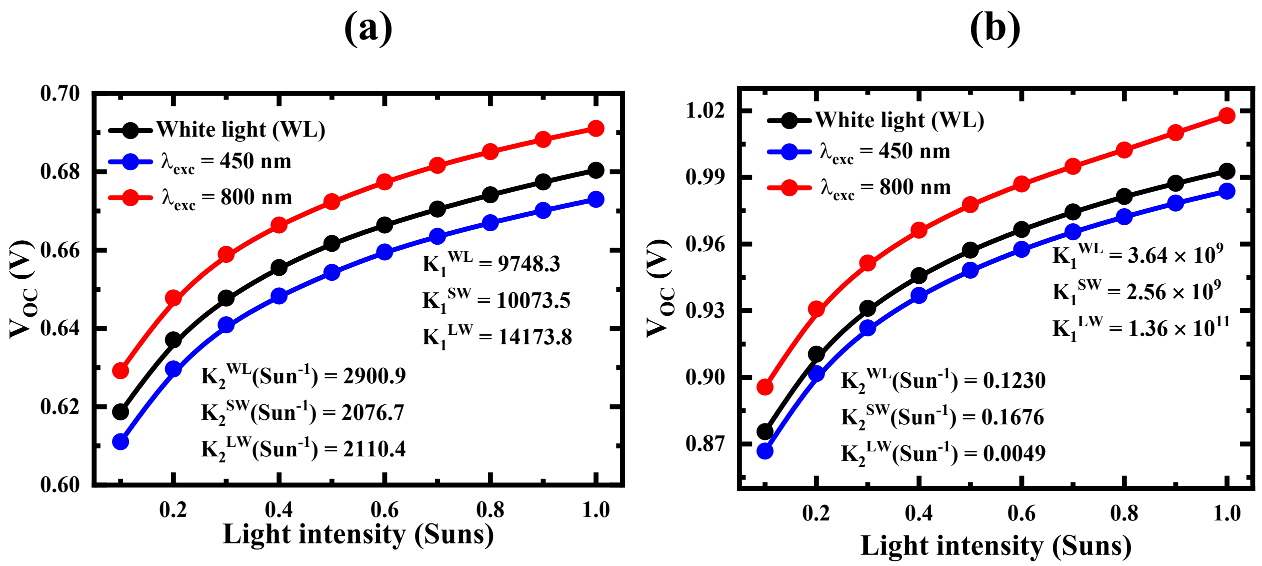

Fig. 1. Light intensity dependent Voc for (a) **n-ZnO/p-MoTe$_2$ (b) n-ZnO/p-MoTe$_2$/ p$^+$-N:Cu$_2$O** device with different excitation wavelength of white light (WL), λexc = 450 nm, and λexc = 800 nm at constant temperature of 300 K.

Table 1 reveals that the recombination coefficient and rate in the depletion region and at the back interface, along with the SRV at the back interface for n-ZnO/p-MoTe$_2$, are notably poor. However, by integrating a 100 nm thick N:Cu$_2$O layer with n-ZnO/p-MoTe$_2$, forming an n-ZnO/p-MoTe$_2$/p+-N:Cu$_2$O structure, there is a significant reduction in the recombination coefficient in the depletion region and at the back interface, from 1.1×10^8 cm^{-2}s^{-1} to 7.1×10^6 cm^{-2}s^{-1} and 1.6×10^3 cm^{-2}s^{-1} to 1.3×10^{-3}, respectively. Consequently, the recombination rate in the depletion region and at the back interface is suppressed from 2.77×10^{16} cm^{-2}s^{-1} to **1.75** $\times 10^{15}$ and 3.98×10^{11} cm^{-2}s^{-1} to 3.35×10^5, respectively. Additionally, the SRV at the back interface is decreased from 200 cm/s to 1.69×10^{-3} cm/s by adding the N:Cu$_2$O BSF layer. These findings imply that the electric field at the p-MoTe$_2$/p$^+$-N:Cu$_2$O interface enhances hole transport from the MoTe$_2$ absorber layer to the back contact via the N:Cu$_2$O-BSF layer, mitigating the flow of minority carriers (electrons) towards the p-MoTe$_2$/p$^+$-N:Cu$_2$O junction, thus reducing the carrier recombination rate at the device's rear side.

Table 1: Extracted values of K$_1$ and K$_2$ from **Fig. 1** and recombination coefficient for MoTe$_2$ based PVSCs with and without N:Cu$_2$O back surface field (BSF) layer. Here R_0^d, $R_0^{i,b}$, R_d, $R^{i,b}$, and S_e^b are calculated at bias voltage of 1.0 V.

Condition	**K_1^{SW}**	**K_1^{LW}**	**K_1^{WL}**	**K_2^{SW}**	**K_2^{LW}**	**K_2^{WL}**	**R_0^d (cm^{-2}s^{-1})**	**$R_0^{i,b}$ (cm^{-2}s^{-1})**	**R^d (cm^{-2}s^{-1})**	**$R^{i,b}$ (cm^{-2}s^{-1})**	**S_e^b (cm/s)**
without N:Cu$_2$O-BSF layer	10073	14173.8	9748.3	2076.7	2110.4	2901	1.1×10^8	1.6×10^3	2.77×10^{16}	3.98×10^{11}	200
with N:Cu$_2$O-BSF layer	2.56×10^9	1.36×10^{11}	3.64×10^9	0.1676	0.0049	0.123	7.1×10^6	1.3×10^{-3}	1.75×10^{15}	3.35×10^5	1.69×10^{-3}

REFERENCES

1. S. Paul, S. Grover, I. L. Repins, B. M. Keyes, M. A. Contreras, K. Ramanathan, R. Noufi Z. Zhao, F. Liao, and J. V. Li, Analysis of Back-Contact Interface Recombination in Thin-Film Solar Cells, IEEE J. Photovoltaics 8(3) (2018) 871–878.