engineering proceedings

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*Proceeding Paper*

# Unveiling Surface Recombination Velocity Influence on the Device Characteristics for the Formamidinium Perovskite Solar Cell †

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† Presented at the 7th International Electrical Engineering Conference, Karachi, Pakistan, 25–26 March 2022.

**Abstract:** Herein, we numerically elucidate the effect of varying surface recombination velocity ($S_{rv}$) at the front and back metal contact on the device performance for our reported lead-free formamidinium tin triiodide ($FASnI_3$) perovskite solar cell. The $S_{rv}$ is generally contemplated as a trivial non-radiative recombination loss factor but determinately impacts the characteristics of the solar cell. Given that, we simultaneously varied the $S_{rv}$ at the back and front metal contacts in the range of $1 \times 10^1$–$1 \times 10^7$ cm/s. Such values for $S_{rv}$ can be realized by ideally passivating the perovskite film and with passivated perovskite films or metallic contact resistive nature. It was inferred that at $S_{rv}$ of $1 \times 10^7$ cm/s, the device efficiency was 21.24% and was steeply increased to 21.42% after decreasing the $S_{rv}$ rate to $1 \times 10^1$ cm/s, revealing that recombination losses are enhanced at a higher $S_{rv}$ rate because of increased carrier recombination at the defect surface, thereby reducing the efficiency and overall performance of the solar cell.

**Keywords:** perovskite solar cell; surface recombination velocity; device performance; numerical investigation

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**Citation:** Saeed, F.; Rehman, T.U.; Zohaib, A.; Farid, A.; Khan, M.H.; Khan, M.A.; Tauqeer, H.A.; Idrees, A. Unveiling Surface Recombination Velocity Influence on the Device Characteristics for the Formamidinium Perovskite Solar Cell. *Eng. Proc.* **2022**, *20*, 4. https://doi.org/10.3390/engproc2022020004

Academic Editor: Saad Ahmed Qazi

Published: 27 July 2022



## 1. Introduction

Among emerging photovoltaic technology, solar cells based on perovskite material (materials of the type $ABX_3$) have attracted enormous attention due to their favorable optoelectronic properties, low fabrication cost, and potential of attaining high efficiency ($\eta$) except the downside of stability [1–3]. The state of the art lab-scale fabricated $\alpha$-$FAPbI_3$ perovskite solar cell characterized by pseudo halide engineering holds the encouraging $\eta \sim 25.6\%$ [4]. Apart from this, non-radiative recombination losses are inevitable in solar cells and more readily emerge in perovskite solar cells due to the ionic nature of perovskite material [5].

Here, we focused on discussing the impact of surface recombination velocity ($S_{rv}$) (one of the non-radiative recombination losses) for the perovskite solar cell. $S_{rv}$ is the rate at which excess minority carriers recombine at the surface (or interface) analogue to the minority carrier lifetime in the bulk of the semiconductor layer [5]. High $S_{rv}$ and low minority carrier lifetime are combined to reduce the carrier collection probability and decline the η [5,6]. The device needs careful optimization in relation to these factors to achieve desirable output characteristics.

Various studies, including numerical and practical investigations, have explored the impacts $S_{rv}$ on the output electrical characteristics, the carrier lifetime, the diffusion length, the collection probability of carriers, and the recombination rate of the solar cells [5–13]. We hereby focused on finding the degree to which $S_{rv}$ influences our recently reported $FASnI_3$ perovskite solar cell [14], wherein we detailed in-depth investigation on the effect of defect density, grain boundaries, and gradient doping on the performance of the solar. Further details to ascertain the likely impact of $S_{rv}$ for the perovskite solar cell are comprehensively provided in this study in the subsequent sections.

## 2. Materials and Methods

We employed a SCAPS-1D environment to perform drift–diffusion simulations for investigating the $S_{rv}$ influence on device characteristics. The perovskite solar cell is the architecture of FTO-etched glass/graphene nano-composites doped with $TiO_2/FASnI_3$/Spiro OmeTAD/Au back metal contact, as depicted in Figure 1a. The material parameters for the simulation can be obtained from the [14]. The device has an open-circuit voltage ($V_{oc}$) of 0.984 V, a short-circuit current density ($J_{sc}$) of 30.235 mA/cm$^2$, a fill factor (FF) of 74.07%, and η of 21.24%. The current–voltage characteristics of the solar cell under AM 1.5G one-sum illumination conditions are depicted in Figure 1b, while the external quantum efficiency is shown in Figure 1c. For investigating the $S_{rv}$, we assumed that $S_{rv}$ is identical at the front and back metal contacts. This assumption is in line with practical realizations [7]. The $S_{rv}$ was varied in the range of $1 \times 10^1$–$1 \times 10^7$ cm/s. The lower values of $S_{rv}$ can be perceived for the encapsulated and passivated perovskite solar cell, while un-passivated perovskite solar cells usually exhibit higher $S_{rv}$ values [15]. Further, it was noticed that devices with metallic contact generally exhibit $S_{rv} > 1 \times 10^5$ cm/s. This study covers all these scenarios and discusses the impact of $S_{rv}$ on the output characteristics, generation–recombination profiles, and quantum efficiency of the solar cell in the later sections.

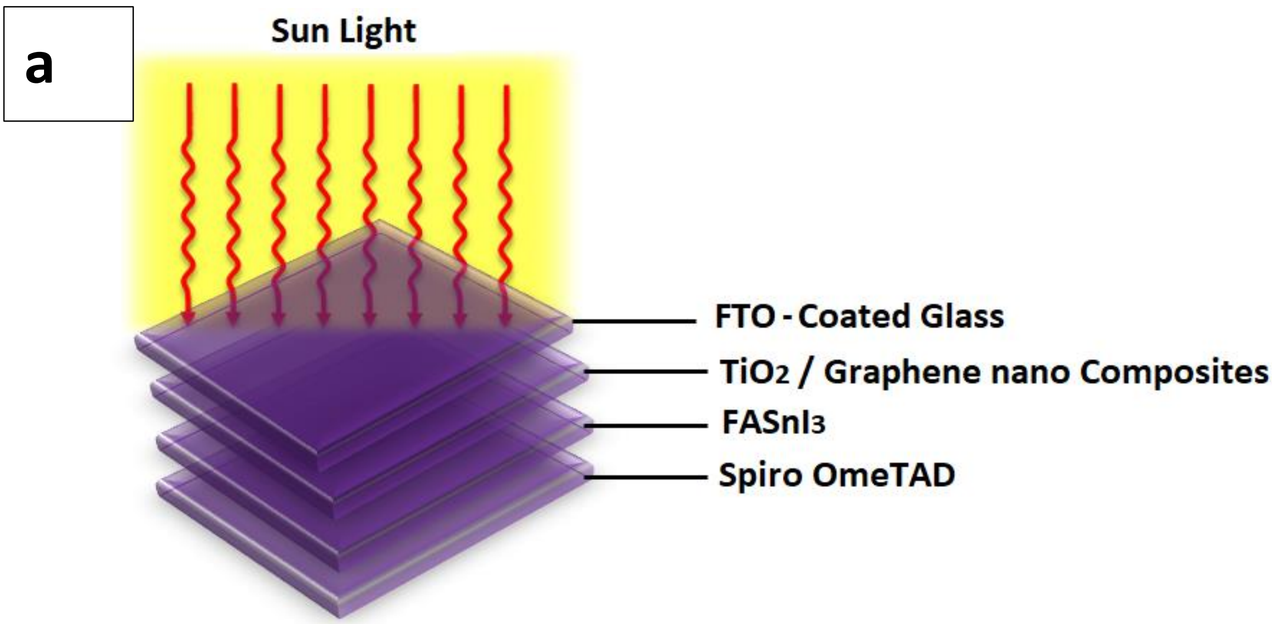


**Figure 1.** *Cont.*

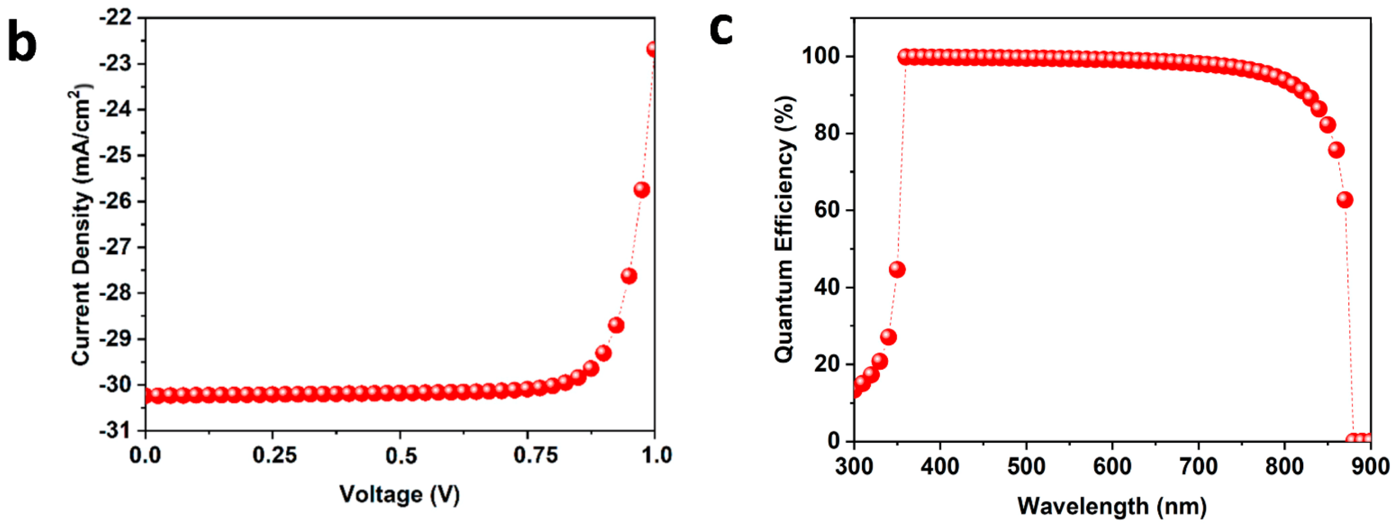


**Figure 1.** (**a**) The structure of the considered perovskite solar cell; (**b**) current density–voltage curve of the solar cell; (**c**) quantum efficiency of the solar cell.

## 3. Results and Discussion

### *3.1. Surface Recombination Velocity Effect on Current–Voltage Characteristics*

As discussed earlier, $S_{rv}$ is the rate at which excess minority carriers recombine at the surface. The mathematical expression relating $S_{rv}$, surface recombination rate ($R_{srv}$), excess minority carriers ($\Delta n$ or $\Delta p$), and carrier lifetime ($\tau$) are given by Equation (1) [15]. This tells us that an increase in $S_{rv}$ results in increased $R_{srv}$, reducing the carrier lifetime as well as the diffusion length according to $L_d = \sqrt{D \times \tau}$ [16], wherein $L_d$ = the diffusion length and $D$ = the diffusion coefficient. Further, the relationship between $J_{sc}$ and $L_d$ and $V_{oc}$ and $L_d$, can be given by Equations (2) and (3), respectively [16,17]. In summary, the relation among these implications can be related as $S_{rv} \propto R_{srv} \propto \frac{1}{\tau} \propto \frac{1}{L_d} \propto \frac{1}{J_{sc}} \propto \frac{1}{V_{oc}}$.

$$S_{rv} = \frac{R_{srv}}{\Delta n} = \frac{1}{\tau_n} \text{ or } S_{rv} = \frac{R_{srv}}{\Delta p} = \frac{1}{\tau_p} \tag{1}$$

$$J_{sc} \approx qGL_d \tag{2}$$

$$V_{oc} = \frac{K_B T}{q} \ln\left(\frac{Jsc}{J_o} + 1\right) \text{ and } J_o \approx \frac{qDn_i^2}{L_d N} \tag{3}$$

In the above expressions, $q$ = the charge, $G$ = the illumination, $n_i$ = the intrinsic carrier concentration, $N$ = the majority carrier dopant concentration, $T$ = the room temperature in Kelvin, and $K_B$ = the Boltzmann constant. The current–voltage curves for varying $S_{rv}$ values from $1 \times 10^1 - 1 \times 10^7$ cm/s for the perovskite solar cell are illustrated in Figure 2a. It can be observed that a decrease in $S_{rv}$ values enhanced the maximum voltage/current points, $V_{oc}$ and $J_{sc}$, of the perovskite solar cell. Figure 2c provides further detailed insight on output parameters extracted from the current–voltage curves shown in Figure 2a. At $S_{rv} = 1 \times 10^7$ cm/s, $V_{oc}$ and $J_{sc}$ were 0.948 V and 30.235 mA/cm$^2$, respectively, and were noticeably improved to 0.9505 V and ~30.485 mA/cm$^2$ as $S_{rv}$ dropped to $1 \times 10^1$ cm/s. The maximum FF was obtained at $S_{rv}$ of $\left(1 \times 10^5 = 1 \times 10^7\right)$ cm/s. Further, η was 21.24% at $1 \times 10^7$ cm/s and steeply increased to 21.42% as we decreased the $S_{rv}$ to $1 \times 10^1$ cm/s. The improvement in device parameters on lowering the $S_{rv}$ corroborates the mitigation of dangling bonds (or the breakdown of the atomic lattice to prompt defect states in energy levels) at lower $S_{rv}$ values and vice versa [12–15].

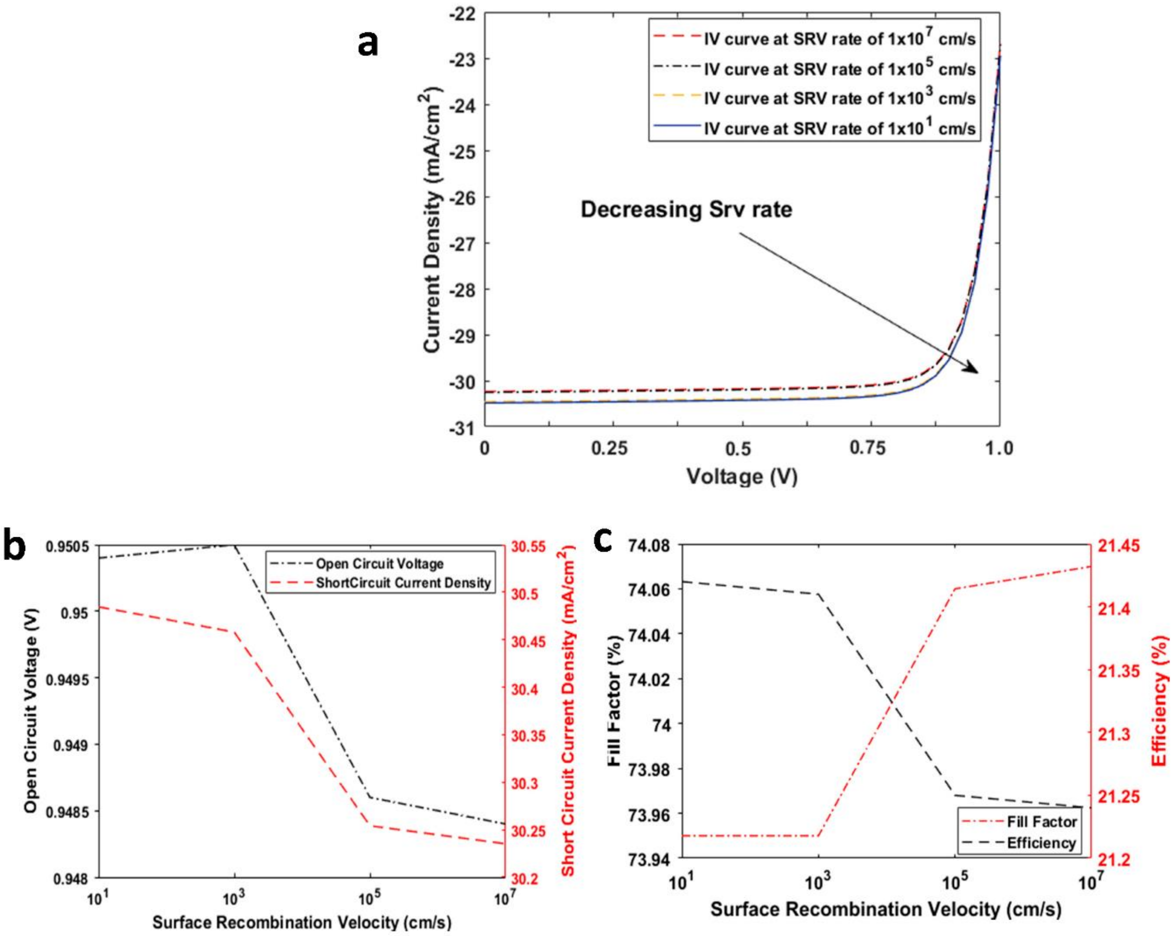


**Figure 2.** Impact of varying surface recombination velocity on the (**a**) current–voltage curves; (**b**) open-circuit voltage and short-circuit current density; and (**c**) fill factor and efficiency of the solar cell.

### *3.2. Surface Recombination Velocity Effect on Generation/RecmobinationRate*

The deterministic impact of $S_{rv}$ on the generation–recombination profile for the perovskite solar is illustrated in Figure 3. The total carrier generation rate $(G_t)$ across all the layers was $\sim 1.68 \times 10^{24}$ $cm^{-3}s^{-1}$ and was the same for all $S_{rv}$ rates. This is because the carrier generation rate is primarily dependent on the incident light intensity. However, the total carrier recombination $(R_t)$ was highest when $S_{rv}$ was $1 \times 10^7$ cm/s and decreases alongside the set minimum boundary value for $S_{rv}$. The $R_t$ was $\sim 2.818 \times 10^{23}$ $cm^{-3}s^{-1}$, $\sim 2.811 \times 10^{24}$ $cm^{-3}s^{-1}$, $\sim 2.787 \times 10^{24}$ $cm^{-3}s^{-1}$, and $\sim 2.784 \times 10^{24}$ $cm^{-3}s^{-1}$ at $S_{rv}$ values of $1 \times 10^7$ cm/s, $1 \times 10^5$ cm/s, $1 \times 10^3$cm/s, and $1 \times 10^1$ cm/s, respectively. This is because with the increase in $S_{rv}$, the minority carrier lifetime and diffusion length decrease due to the emergence of defect states, thereby increasing the recombination rate of the carriers and vice versa [15–17].

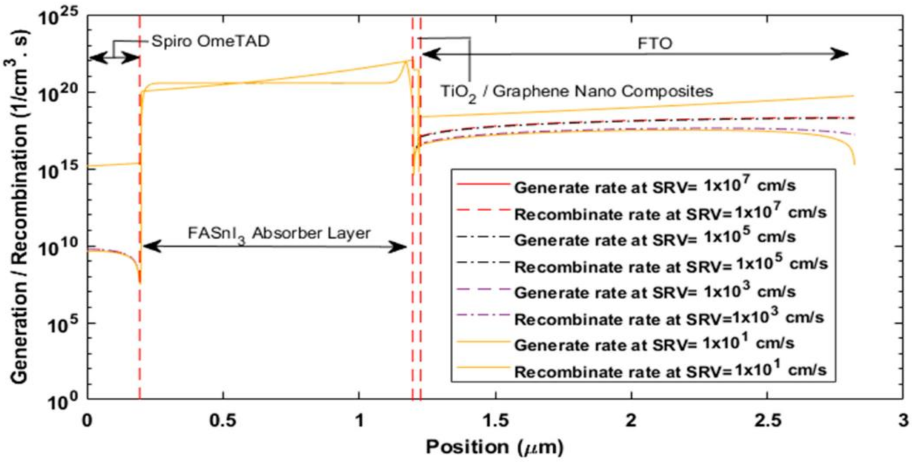


**Figure 3.** Impact of varying surface recombination velocity on the generation–recombination rate of the solar cell.

### 3.3. Surface Recombination Velocity Effect on External Quantum Efficiency

The external quantum efficiency as a function of incident light wavelength for the perovskite solar cell is also observed to be influenced by the variation in $S_{rv}$, as shown in Figure 4. It can be noticed that the device quantum efficiency profile improved as we decreased the $S_{rv}$ from $10^7$–$10^1$ cm/s. The prominent difference in the quantum efficiency is easily noticeable for the wavelengths $\geq$ 300 nm and <360 nm. The quantum efficiency at the inception (at an incident light wavelength of 300 nm) was ∼13.3% and 18.9% for $S_{rv}$ values of $1 \times 10^7$ cm/s and $1 \times 10^5$ cm/s, respectively. The quantum efficiency unprecedently enhanced to $\geq$79% as $S_{rv}$ decreased beyond the $1 \times 10^3$ cm/s. This is because the quantum efficiency of the solar cell is highly deterministic on the proportion of light being transmitted (and absorbed) or reflected from the surface of the solar cell [8]. In the current context, the decrease in quantum efficiency at higher $S_{rv}$ values can be related to the inability of perovskite solar cells to harvest incident photons because of inappropriate surface texturing and defects at the interface of metal contacts and perovskite film [5,15–17].

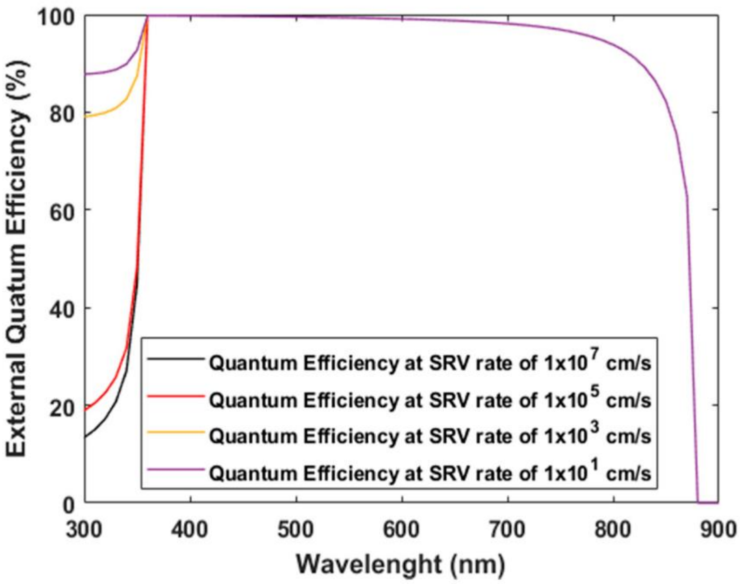


**Figure 4.** Impact of varying surface recombination velocity on the external quantum efficiency of the solar cell.

## 4. Conclusions

The computational investigation demonstrated that $S_{rv}$ can strongly influence the carrier generation–recombination rate, quantum efficiency, power conversion efficiency, and overall device performance. Higher $S_{rv}$ results in reduced increases in the carrier recombination before collection at the respective contacts, as well as decreased quantum efficiency of the solar cell, and vice versa. The η of the device is enhanced to 21.42% from the reported 21.24% on decreasing the $S_{rv}$ from $1 \times 10^7$ cm/s and $1 \times 10^1$ cm/s, respectively. So, the adverse effects of $S_{rv}$ can be controlled by carefully passivating the surface (and interface) and the synthetization of reduced defect perovskite films.

**Author Contributions:** Conceptualization, F.S.; methodology, F.S., T.U.R., A.Z., A.F., M.H.K., M.A.K., H.A.T. and A.I.; software, F.S., T.U.R., A.Z., A.F., M.H.K., M.A.K., H.A.T. and A.I.; writing—original draft preparation, F.S., T.U.R., A.Z., A.F., M.H.K., M.A.K., H.A.T. and A.I.; Writing-reviewing and editing, F.S. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research received no external funding.

**Conflicts of Interest:** The authors declare no conflict of interest.

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