COMMENT

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Comment on "Improving the efficiency of a CIGS solar cell to above 31% with Sb_2S_3 as a new BSF: a numerical simulation approach by SCAPS-1D" by M. F. Rahman and S. Goumri-Said et al., RSC Adv., 2024, 14, 1924

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It was reported in early 2024 that a single-junction 1.1 eV bandgap copper indium gallium selenide (CIGS) solar cell can achieve actual power conversion efficiency up to 40.70%, open circuit voltage up to 1.330 V, and fill factor up to 90.55% at 300 K when the solar cell is irradiated by the air mass 1.5 global (AM1.5G) solar spectrum (M. F. Rahman *et al.*, *RSC Adv.*, 2024, **14**, 1924–1938). These simulated solar cell performance parameters exceed the ideal detailed balance-limiting power conversion efficiency, open circuit voltage, and fill factor of a 1.1 eV bandgap single-junction solar cell.

1 Introduction

Based on simulations run with a conventional one-dimensional drift-diffusion solar cell modeling program, SCAPS-1D, Rahman *et al.* reported that a conventional 1.1 eV bandgap copper indium gallium selenide (CIGS) solar cell can achieve actual air mass 1.5 global (AM1.5G) power conversion efficiency η up to 40.70%, open circuit voltage V_{oc} up to 1.330 V, and fill factor FF up to 90.55%.[1] The device design that was simulated contains an aluminum (Al) top grid contact, a 50 nm thick fluorine-doped tin oxide (FTO) layer, a 50 nm thick tin disulfide (SnS_2) layer, a 1.1 eV bandgap CIGS primary absorbing layer with thickness up to 3000 nm, a 200 nm thick antimony trisulfide (Sb_2S_3) layer, and a nickel (Ni) rear contact. A schematic of the solar cell proposed by Rahman *et al.* is shown in Fig. 1.
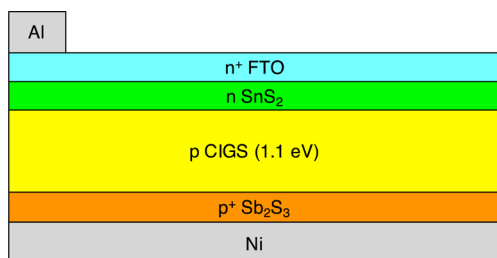
2 Discussion

Before modeling any type of solar cell with a standard drift-diffusion computer program, it is helpful to determine its theoretical efficiency limit. In the field of photovoltaics, this is typically accomplished by using the principle of detailed balance to calculate the ideal limiting efficiency.[2,3] The benefit of this approach is that the detailed balance formalism allows for a fundamental determination of the efficiency limit of a solar cell independent of specific device design features such as the thickness of individual layers, the dopant concentrations, and the contact metal work functions. Moreover, the only sink for photogenerated electron and hole recombination at steady-state and open circuit is the necessary radiative recombination
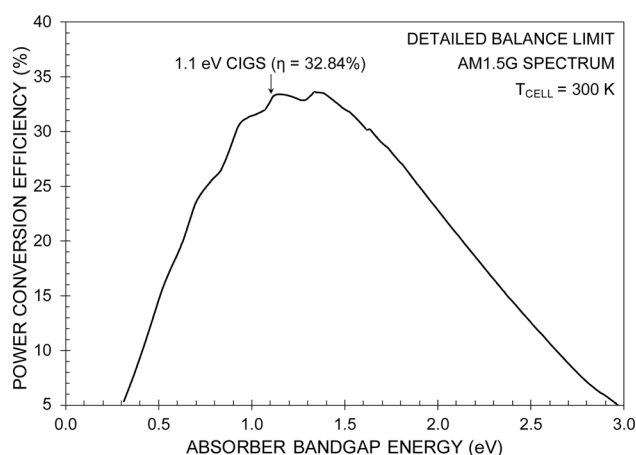

Fig. 1 Cross section view of 1.1 eV bandgap CIGS solar cell.

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Fig. 2 Detailed balance-limiting power conversion efficiency.

Table 1 Detailed balance-limiting performance of a 1.1 eV CIGS solar cell irradiated by the AM1.5G spectrum with $T_{cell} = 300$ K[a]

Case	Absorber	E_g (eV)	J_{sc} (mA cm^{-2})	V_{oc} (V)	V_{mp} (V)	J_{mp} (mA cm^{-2})	FF (%)	η (%)
1	CIGS	1.1	44.23	0.8590	0.7676	42.79	86.46	32.84
2	CIGS	1.1	34.55	0.8526	0.7614	33.42	86.38	25.44

[a] Key: E_g is bandgap energy, J_{sc} is short circuit current density, V_{oc} is open circuit voltage, V_{mp} is max power point voltage, J_{mp} is max power point current density, FF is fill factor, and η is power conversion efficiency. Note: "Case 1" assumes maximum AM1.5G J_{sc} whereas "Case 2" assumes a reduced J_{sc}. Note: Rahman et al. reported V_{oc} up to 1.330 V, FF up to 90.55%, and η up to 40.70%.

whereas the undesirable nonradiative Auger and Shockley–Read–Hall recombination are not considered. A plot of the detailed balance-limiting power conversion efficiency η of single-junction solar cells, as a function of absorber bandgap energy, is shown in Fig. 2.

The equations required to calculate the detailed balance-limiting performance are listed next. The open circuit voltage is expressed as $V_{oc} = E_g/q - (kT/q)\ln[(2\pi q E_g^2 kT)/(h^3 c^2 J_{sc})]$, where E_g is the bandgap energy, q is the electron charge, k is the Boltzmann constant, T is the cell temperature, h is the Planck constant, and c is the speed of light in vacuum. The max power point voltage is expressed as $V_{mp} \approx V_{oc} - (kT/q)\ln[1 + (qV_{oc}/kT)]$. The max power point current density is expressed as $J_{mp} = J_{sc}/[1 + (kT/qV_{mp})]$. The fill factor is expressed as FF $= (J_{mp}V_{mp})/(J_{sc}V_{oc})$. The power conversion efficiency is expressed as $\eta = P_{out}/P_{in}$, where $P_{out} = J_{mp}V_{mp}$ and $P_{in} = 0.1$ W cm^{-2} (AM1.5G irradiance).

The maximum available short circuit current density J_{sc} of a 1.1 eV bandgap semiconductor is 44.23 mA cm^{-2} when considering the AM1.5G solar spectrum. In Table 1, the detailed balance-limiting V_{oc}, FF, and η are shown for two cases. In Case 1, the maximum AM1.5G spectrum J_{sc} of 44.23 mA cm^{-2} is considered. In Case 2, a reduced J_{sc} of 34.55 mA cm^{-2} is considered. This smaller J_{sc} value was chosen to match the peak J_{sc} reported by Rahman et al.[1] Nonetheless, in both cases the detailed balance-limiting V_{oc}, FF, and η are less than the peak values reported by Rahman et al.[1] In particular, refer to the simulated V_{oc}, FF, and η values reported in Section 4.3 on p. 1932 as well as Fig. 4 on p. 1929, Fig. 6 on p. 1931, and Fig. 7 on p. 1932 of the article by Rahman et al.[1] Not only do these figures show simulated peak V_{oc}, FF, and η exceeding the ideal detailed balance limit, they also show that these simulated peak performance parameters occur when the bulk and interface defect concentrations are the largest of the range of values that were simulated by Rahman et al.[1] Note, too, that the peak V_{oc} (1.330 V) reported by Rahman et al. exceeds the bandgap-equivalent voltage ($E_g/q = 1.1$ V) of the CIGS absorber.

3 Conclusion

In summary, Rahman et al. reported unrealistic values of open circuit voltage V_{oc}, fill factor FF, and power conversion efficiency η of a 1.1 eV CIGS single-junction solar cell even though their proposed solar cell is a conventional device that was modeled with standard drift-diffusion physics. More to the point, in their device simulations, Rahman et al. did not consider hot carrier collection or some other attribute that might result in actual open circuit voltage and power conversion efficiency exceeding the detailed balance-limiting open circuit voltage and power conversion efficiency.

Author contributions

Alexander P. Kirk: conceptualization, formal analysis, visualization, writing – original draft, review & editing.

Conflicts of interest

There are no conflicts of interest to declare.

References

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