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Electronic Supplementary Information

Energy-Yield Prediction for II-VI-based Thin-Film Tandem Solar Cells

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Tandem Radiative Efficiency Limit with One-Diode Model

In this ideal optical model, photons with $E_{ph} > E_{g,top}$ are fully absorbed and collected by the top cell while the remaining light with $E_{g,top} > E_{ph} > E_{g,bot}$ is fully absorbed and collected by the bottom cell. E_{ph} is the photon energy, while $E_{g,top}$ and $E_{g,bot}$ are the top and the bottom cell E_g, respectively.[1,2] The luminescent coupling among the sub-cells is neglected because the effect on sub-cell current density is small, as has been previously shown.[1] The one-diode models used to calculate the *J*-*V* curves are adopted from the literature.[1,3] We assume that the recombination mechanism in a solar cell with known E_g is radiatively-limited:

$$J_{\mathrm{dark}}(V) = J_{0,\mathrm{SQ}}(exp(qV/kT) - 1) \tag{1}$$

$$J_{0,\mathrm{SQ}} = 2q \int_{\frac{qE_g}{h}}^{\infty} \frac{2\pi v^2}{c^2(exp(hv/kT)-1)} dv \tag{2}$$

where J_{dark} is the dark current, V is the operating voltage, $J_{0,SQ}$ is the radiative dark current given by the detailed-balance, or SQ limit, q is the elementary charge, k is Boltzmann's constant, T is operating temperature at 25 ^{o}C, h is Planck's constant, c is the speed of light, and v is the state transition energy multiplied by q/h. [1,3] We can use the $J_{0,SQ}$ to construct the sub-cell current-density-voltage J-V curves:

$$J_{\mathrm{top}}(V_{\mathrm{top}}) = J_{\mathrm{sc,top}} - J_{\mathrm{0,SQ,top}}(exp(qV_{\mathrm{top}}/kT) - 1) \quad (3)$$

$$J_{\mathrm{bot}}(V_{\mathrm{bot}}) = J_{\mathrm{sc,bot}} - J_{\mathrm{0,SQ,bot}}(exp(qV_{\mathrm{bot}}/kT) - 1) \quad (4)$$

where J_{top}, J_{bot}, V_{top}, and V_{bot} are the current densities and operating voltage of the top and the bottom cells, respectively. The radiative efficiency limits of 4T (η_{4T}, independently operated sub-cells) and 2T (η_{2T}, series-connected sub-cells) tandems are then calculated using the formulae:

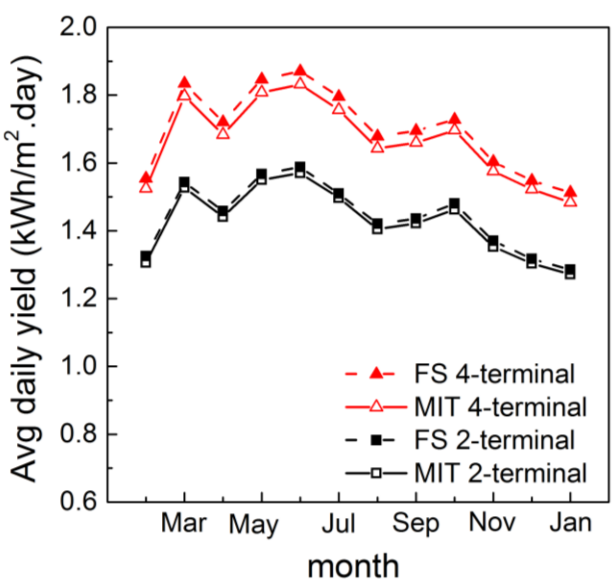
$$\eta_{\mathrm{4T}} = \left(max(J_{\mathrm{top}}V_{\mathrm{top}}) + max(J_{\mathrm{bot}}V_{\mathrm{bot}})\right)/P_{\mathrm{in}} \quad (5)$$

$$\eta_{\mathrm{2T}} = max\left(J\left(V_{\mathrm{top}}(J) + V_{\mathrm{bot}}(J)\right)\right)/P_{\mathrm{in}} \quad (6)$$

where P_{in} is the incident sunlight power under AM1.5G.

Energy-Yield Model 3 Validation using Published GaAs-Si Tandem Device Physics Model

In order to test the validity of the semi-empirical energy-yield model (Model 3), we compare the performance of the model to a previously published energy-yield model developed by Liu et.al.[4] The same optical stack (layer material (*n*,*k*) data & thicknesses) to calculate the optical absorption in the layers in the two models. Because $EQE(\lambda)$ calculation for Model 3 is only valid for thin-film devices, the actual $EQE(\lambda)$ for the bottom Si cell of Model 3 (FS) is taken from the PC1D device physics simulator model calculated by the MIT model.[4] The same annual sunlight input spectrum for Singapore is used for the two models. Apart from that, the energy-yield calculation for the semi-empirical FS model is performed independently from the MIT device physics model.[4] Energy-yield output comparison for the two models are shown in **Supplementary Figure 1**, showing that the semi-empirical FS model works just as well as the numerical device physics MIT model.



Supplementary Figure 1. Comparison of average daily energy yield for 4T (red triangles) and 2T (black squares) GaAs/Si tandem[4] solar cells under annual Singapore spectrum, modeled using PC1D device physics simulator (MIT)[4] and semi-empirical Model 3 of this paper (FS). There is a negligible difference of energy-yield result between the two models, but the semi-empirical model is several orders of magnitudes faster than a full-fledged device physics simulator model.

Thin-Film Optical Modeling for Energy-Yield Model 3

Optical absorption $A(\lambda)$ for each sub-cell is calculated using a transfer matrix method (TMM) simulation.[5] We use published (n,k) optical data for GaSb,[6] CIGS,[7] CdS,[8] ITO,[5] Mo,[9] and EVA,[10] while (n,k) for the remaining layers are measured by First Solar. The (n,k) profile for a hypothetical high-E_g II-VI top absorber layer (only used in Architecture B) is obtained by shifting the (n,k) profile for CdTe up by 0.23 eV in the energy domain, which enables us to J-match the tandem sub-cells in Architecture B. We extract J_{sc} from the external quantum efficiency $EQE(\lambda)$, assuming $EQE(\lambda) = A(\lambda)$.

Series and Shunt Resistance Fitting for Energy-Yield Model 3

Internal series and shunt resistance values R_s and R_{sh} of sub-cells are fitted and extracted from the literature and summarized in **Table 4**.[11–13] For the fitting routine we use the equations[14]:

$$J_0 = J_{\mathrm{sc,1-sun}} / \left(exp\left(\frac{qV_{\mathrm{oc,1-sun}}}{nkT}\right) - 1 \right) \tag{7}$$

$$J(V) = J_{\mathrm{sc}} - J_0 \left(exp\left(\frac{q(V+J(V)R_{\mathrm{s}})}{nkT}\right) - 1 \right) - \frac{(V+J(V)R_{\mathrm{s}})}{R_{\mathrm{sh}}} \tag{8}$$

where $J_{sc,1\text{-}sun}$ is the calculated J_{sc} of the sub-cell under AM1.5G illumination. We note that while the J_0 calculation in **Equation 7** is a simplified form that ignores R_s and R_{sh}, the resulting *J*-*V* curve calculated using **Equation 8**, which includes R_s and R_{sh}, is a close fit to *J*-*V* curve of the cell found in literature.

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