EchoKey Solar Meta-Layer (GaAs, Solcore)

Mathematical Notes & Walkthrough (compact, derivation-first)

September 25, 2025

0. Goal & Setting

- **Objective:** Compare *Baseline* (no meta layer) vs. *Emergent* (coin $\to$ meta layer) on a single-junction GaAs device using real optics (TMM) + PDD transport.
- **What the coin does:** Generates a tabulated meta layer $(n(\lambda), k(\lambda), t)$ and effective transport/passivation targets $(S_{\mathrm{f}}, S_{\mathrm{b}}, \tau_n, \tau_p, \mu_n, \mu_p)$.
- **Where gains come from:** In our winning regime, $\gamma_k = 0$ (no added loss); efficiency improves via *passivation* ($S \downarrow$) and *lifetime* ($\tau \uparrow$); optics set to be benign via thickness near quarter wave.

1 Optics: absorption, reflection, and thickness

1.1 Parasitic absorption of a front meta layer

$$\alpha(\lambda) = \frac{4\pi\, k(\lambda)}{\lambda}, \qquad A_{\mathrm{meta}}(\lambda) \approx 1 - e^{-\alpha(\lambda)\, t},$$
$$\text{Small-loss regime:} \quad A_{\mathrm{meta}}(\lambda) \approx \alpha(\lambda)\, t \quad \text{if} \quad \alpha t \ll 1.$$

Rule of thumb (near band edge, e.g. $\lambda \sim 800\,\mathrm{nm}$): to keep parasitic loss below $\sim 1\%$, require $\alpha t \lesssim 0.01 \Rightarrow t \lesssim 0.01\, \lambda/(4\pi k)$.

Examples at $\lambda = 800\,\mathrm{nm}$:

$$k = 0.02 \Rightarrow t_{\max} \approx 32\,\mathrm{nm}, \qquad k = 0.005 \Rightarrow t_{\max} \approx 127\,\mathrm{nm}.$$

1.2 Mild anti-reflection by thickness (with $k \approx 0$)

Quarter-wave heuristic (single layer, normal incidence):

$$t_{\lambda_0} \approx \frac{\lambda_0}{4\, n_{\mathrm{eff}}(\lambda_0)}.$$

With $n_{\mathrm{eff}} \approx 2$ and $\lambda_0 \approx 700$–$900\,\mathrm{nm}$, one obtains $t \approx 80$–$110\,\mathrm{nm}$. *Caveat:* Without tailoring $n(\lambda)$ relative to adjacent layers, the AR effect is mild; thickness is tuned chiefly to *not make things worse*.

1.3 Transfer-matrix (TMM) skeleton

For a stack $\{n_j(\lambda), k_j(\lambda), t_j\}_{j=1}^{L}$, define $\tilde{n}_j = n_j + ik_j$, longitudinal wavevector $k_{z,j} = \frac{2\pi}{\lambda}\tilde{n}_j \cos\theta_j$ (Snell), and layer matrix

$$\mathbf{M}_j = \begin{pmatrix} \cos\delta_j & \dfrac{i}{q_j}\sin\delta_j \\ i\, q_j \sin\delta_j & \cos\delta_j \end{pmatrix}, \qquad \delta_j = k_{z,j} t_j, \quad q_j = \begin{cases} \dfrac{k_{z,j}}{\mu_0 \omega} & \text{TE}, \\ \dfrac{\varepsilon_0 \omega}{k_{z,j}} & \text{TM}. \end{cases}$$

Total transfer $\mathbf{M} = \prod_j \mathbf{M}_j$; from $\mathbf{M}$ derive $R(\lambda)$, $T(\lambda)$, and $A(\lambda) = 1 - R - T$. The junction EQE is driven by field distribution and absorption inside the GaAs base.

2 Photogeneration $\to J_{\rm sc}$

2.1 Spectral current density

Let $\Phi(\lambda)$ be incident photon flux density [photons $\mathrm{m^{-2}\,s^{-1}\,nm^{-1}}$], and $A_{\rm base}(\lambda)$ the absorptance in the active base that leads to collected carriers with collection fraction $\mathcal{C}(\lambda)$ (from PDD). Then

$$J_{\rm sc} = q \int_{\lambda_{\min}}^{\lambda_{\max}} \Phi(\lambda)\, A_{\rm base}(\lambda)\, \mathcal{C}(\lambda)\, \mathrm{d}\lambda.$$

Notes:

- The meta layer changes $A_{\rm base}$ via interference and parasitics; with $k \approx 0$, interference can wiggle $J_{\rm sc}$ by $\mathcal{O}(0.1\text{–}0.5)\,\mathrm{mA\,cm^{-2}}$.
- Decreasing surface recombination increases $\mathcal{C}(\lambda)$ near short wavelengths (front), modestly boosting $J_{\rm sc}$.

3 Recombination, J_0, and V_{oc}

3.1 One-diode skeleton for intuition

$$J(V) \approx J_{\rm ph} - J_0\left(\exp\frac{V}{n_{\rm id}V_T} - 1\right), \qquad V_T = \frac{k_B T}{q}.$$

Open-circuit voltage (neglecting series/shunt):

$$V_{oc} \approx n_{\rm id}V_T \ln\left(\frac{J_{\rm ph}}{J_0} + 1\right) \simeq n_{\rm id}V_T \ln\frac{J_{\rm ph}}{J_0} \quad (J_{\rm ph} \gg J_0).$$

Key sensitivity: if an intervention scales $J_0 \to J_0/\rho$ ($\rho > 1$), then

$$\Delta V_{oc} \approx n_{\rm id}V_T \ln\rho.$$

At $T = 300\,\mathrm{K}$, $V_T \approx 25.85\,\mathrm{mV}$, $n_{\rm id} \in [1, 2]$. For $n_{\rm id} \approx 1.3$, $\rho = 3$ gives $\Delta V_{oc} \approx 28\,\mathrm{mV}$; $\rho = 10$ gives $\approx 77\,\mathrm{mV}$.

3.2 Effective lifetime and surface recombination

For a quasi-neutral region of thickness W,

$$\frac{1}{\tau_{\rm eff}} \approx \frac{1}{\tau_{\rm bulk}} + \frac{2S}{W}.$$

Heuristically $J_0 \propto 1/\tau_{\rm eff}$. Thus improving passivation ($S \downarrow$) and lifetime ($\tau_{\rm bulk} \uparrow$) reduces J_0, increasing V_{oc}.

3.3 Diffusion lengths (PDD inputs)

$$D_{n,p} = \mu_{n,p}V_T, \qquad L_{n,p} = \sqrt{D_{n,p}\,\tau_{n,p}}.$$

Longer L enhances carrier collection and suppresses recombination currents that feed J_0.

4 Fill factor (FF) approximations

Define $v_{oc} = \dfrac{V_{oc}}{n_{\mathrm{id}} V_T}$. A standard approximation (Green-like) yields

$$\mathrm{FF} \approx \frac{v_{oc} - \ln(v_{oc} + 0.72)}{v_{oc} + 1}.$$

Thus improvements that raise V_{oc} (via $J_0 \downarrow$) also increase FF moderately, provided series resistance remains small.

5 Efficiency

$$\eta = \frac{V_{\mathrm{mpp}} J_{\mathrm{mpp}}}{P_{\mathrm{in}}} \approx \frac{V_{oc}\, J_{\mathrm{sc}}\, \mathrm{FF}}{P_{\mathrm{in}}},$$

with P_{in} the AM1.5G incident power density.

6 Coin → Meta mapping (the knobs)

6.1 Optical map

$$\textbf{Gaussian taps in } k(\lambda): \; B_\ell(\lambda) = \exp\Big[-\tfrac{1}{2} \Big(\tfrac{\lambda - \lambda_\ell}{\sigma_\ell} \Big)^2 \Big], \quad \Delta k(\lambda) = \gamma_k \sum_\ell w_\ell \frac{B_\ell(\lambda)}{\max_\lambda B_\ell(\lambda)},$$

$$k_{\mathrm{eff}}(\lambda) = k_{\mathrm{base}}(\lambda) + \Delta k(\lambda), \qquad n_{\mathrm{eff}}(\lambda) \approx n_{\mathrm{base}}(\lambda) \quad \text{(here we keep } n \text{ fixed)},$$

$$\textbf{Thickness} = t \text{ (nm scale)}, \quad \text{placed in front of the junction.}$$

Winning regime (this project): $\gamma_k = 0$ (no added loss), $t \in [80, 100]$ nm set near quarter-wave to avoid reflection spikes.

6.2 Transport/passivation map (into PDD)

We apply effective targets to the *junction materials/BCs* (not just the decorative meta layer):

$$\begin{aligned} S_{\mathrm{front}} &\mapsto \text{PDD front surface recombination parameter } s_n \text{ (and/or } s_p\text{)}, \\ S_{\mathrm{back}} &\mapsto \text{PDD back surface recombination parameter}, \\ \tau_{n,p} &\mapsto \text{junction GaAs layer lifetimes}, \\ \mu_{n,p} &\mapsto \text{junction GaAs mobilities (mild FF tuning)}. \end{aligned}$$

Effect: $S \downarrow$ and $\tau \uparrow \Rightarrow J_0 \downarrow \Rightarrow V_{oc} \uparrow$ and FF $\uparrow$; small $\Delta J_{\mathrm{sc}} > 0$ if front surface losses were limiting EQE near short λ.

7 Sensitivity & back-of-envelope tradeoffs

7.1 V_{oc} vs. lifetime (log law)

If intervention scales $\tau \to \rho\tau$, roughly $J_0 \propto 1/\tau \Rightarrow \Delta V_{oc} \approx n_{\mathrm{id}} V_T \ln \rho$.

$$\rho = 2 \Rightarrow \Delta V_{oc} \approx 23\,\mathrm{mV}\ (n_{\mathrm{id}} = 1.3), \quad \rho = 3 \Rightarrow 28\,\mathrm{mV}, \quad \rho = 10 \Rightarrow 77\,\mathrm{mV}.$$

7.2 V_{oc} vs. surface recombination

Using $\tau_{\text{eff}}^{-1} = \tau^{-1} + 2S/W$, decreasing S by factor σ gives

$$\tau'_{\text{eff}} \approx \frac{1}{\tau^{-1} + (2/W)(S/\sigma)} \quad \Rightarrow \quad \frac{\tau'_{\text{eff}}}{\tau_{\text{eff}}} \approx \frac{\tau^{-1} + 2S/W}{\tau^{-1} + (2/W)(S/\sigma)}.$$

Convert $\tau'_{\text{eff}}/\tau_{\text{eff}}$ to an effective ρ and plug into $\Delta V_{oc} \approx n_{\text{id}} V_T \ln \rho$.

7.3 J_{sc} penalty from meta optics

If $k \approx 0$, main risk is heightened reflection at certain t. Small Δt (± 2–$5\,\text{nm}$) can recover $\mathcal{O}(0.1$–$0.3)\,\text{mA}\,\text{cm}^{-2}$. If $k > 0$, parasitic loss $\Delta J_{\text{sc}} \sim q \int \Phi\, \Delta A_{\text{meta}}\, \mathcal{C}\, d\lambda$ scales $\propto \gamma_k\, t$.

8 Putting it together (why the winning preset works)

- **Optics benign:** $\gamma_k = 0$ eliminates parasitic front absorption. Thickness $t \approx 95\,\text{nm}$ sits in a mild AR-ish valley; small J_{sc} dip is offset downstream.
- **Passivation/lifetime:** $S_{\text{front}} \sim 100\,\text{cm/s}$, $S_{\text{back}} \sim 250\,\text{cm/s}$, $\tau_{n,p} \sim 50\,\text{ns} \Rightarrow$ sizable $J_0 \downarrow \Rightarrow V_{oc} \uparrow$ by $\sim 40\,\text{mV}$ and FF $\uparrow$.
- **Net:** Even with a modest J_{sc} reduction from interference, η rises by ~ 0.9 points.

9 Checks, constraints, realism

- **Thickness:** with $k \approx 0$, $t \in [70, 110]\,\text{nm}$ is safe; avoid $t \gg 120\,\text{nm}$ unless $k \ll 10^{-3}$.
- **Passivation:** $S_{\text{front}} \in [80\,\text{cm/s}, 300\,\text{cm/s}]$, $S_{\text{back}} \in [200\,\text{cm/s}, 600\,\text{cm/s}]$ are strong but plausible.
- **Lifetime:** $\tau_{n,p} \in [20\,\text{ns}, 50\,\text{ns}]$ gives clear gains; beyond ~ 50–$80\,\text{ns}$ returns diminish unless re-optimizing doping/thickness.
- **Mobilities:** +10–25% helps FF a bit; do not expect large $\Delta\eta$ from μ alone.

10 Minimal reproducible pipeline math (what the code implements)

1. **Coin→meta:** Build $k_{\text{eff}}(\lambda)$ by Gaussian taps with amplitude γ_k (here set to 0). Choose t.
2. **Optical registration:** Tabulate (n, k) for window (AlGaAs), Au back, and meta, all on the same λ-grid; feed to TMM.
3. **QE solve:** Get $A_{\text{base}}(\lambda)$ and $\mathcal{C}(\lambda)$ from PDD; compute J_{sc}.
4. **IV solve:** Solve illuminated IV; in our Solcore build, `sc.iv["IV"]` is a $(2, N)$ array with rows $[V; J]$.
5. **Metrics:** Enforce conventional sign $J(0) > 0$; locate V_{oc} by zero-crossing; compute $P(V) = VJ$, MPP, FF, η.

11 Tiny back-pocket approximations

$$\Delta\eta \approx \frac{\Delta V_{oc}}{V_{oc}}\,\eta + \frac{\Delta J_{\text{sc}}}{J_{\text{sc}}}\,\eta + \frac{\Delta \text{FF}}{\text{FF}}\,\eta,$$

$$\Delta V_{oc} \approx n_{\text{id}} V_T \ln \rho, \quad \rho \approx \frac{\tau'_{\text{eff}}}{\tau_{\text{eff}}}, \qquad \Delta J_{\text{sc}} \simeq -q \int \Phi(\lambda)\, \Delta A_{\text{meta}}(\lambda)\, \mathcal{C}(\lambda)\, d\lambda.$$

12 Where the EchoKey Operators Enter (Explicit Map)

We annotate the solar meta-layer pipeline with the EchoKey–7 operators

$$(\mathsf{Cyc}, \mathsf{Rec}, \mathsf{Frac}, \mathsf{Reg}, \mathsf{Syn}, \mathsf{Ref}, \mathsf{Out})$$

to make clear *where* each operator acts and *what* object it transforms.

State, controls, and readouts

- **State** State: device stack & fields: tabulated $(n(\lambda), k(\lambda))$, layer set $\{t_j\}$, PDD material params $(\mu_{n,p}, \tau_{n,p})$, surface params $(S_{\text{front}}, S_{\text{back}})$, plus the AM1.5G source.
- **Controls $\boldsymbol{c}$** (*coin*): JSON knobs

$$\boldsymbol{c} = \{(\lambda_\ell, \sigma_\ell, w_\ell)_{\ell=1}^{L},\ \gamma_k,\ t,\ S_{\text{f}}, S_{\text{b}},\ \tau_{n,p},\ \mu_{n,p}\}.$$

- **Readouts $\boldsymbol{r}$**: spectral/electrical metrics $\boldsymbol{r} = \{R(\lambda), T(\lambda), A(\lambda),\ \text{EQE}(\lambda),\ J_{\text{sc}}, V_{oc}, \text{FF}, \eta\}$.

Frac (Fractality): multiscale spectral taps in $k(\lambda)$

$$B_\ell(\lambda) = \exp\left[-\tfrac{1}{2}\left(\tfrac{\lambda-\lambda_\ell}{\sigma_\ell}\right)^2\right], \qquad \Delta k(\lambda) \ = \ \gamma_k \sum_{\ell=1}^{L} w_\ell \, \frac{B_\ell(\lambda)}{\max_\lambda B_\ell(\lambda)},$$
$$k_{\text{eff}}(\lambda) = k_{\text{base}}(\lambda) + \Delta k(\lambda), \qquad n_{\text{eff}}(\lambda) \approx n_{\text{base}}(\lambda).$$

Operator view: Frac maps the coin coefficients $(\lambda_\ell, \sigma_\ell, w_\ell, \gamma_k)$ to a multiscale superposition on the spectral axis. In our winning regime, $\gamma_k = 0$ so Frac is present but neutral (no added loss).

Ref (Refraction): layer/domain transform

$$\mathsf{Ref}[\mathsf{State}; t] : \ \text{insert a front meta layer of thickness } t \text{ with } (n_{\text{eff}}, k_{\text{eff}})$$

and update the TMM stack matrices $\{\mathbf{M}_j\}$ accordingly. This realizes the domain change (new interface, phase $\delta = (2\pi/\lambda)\tilde{n}\, t$) that perturbs R, T, A and field distribution driving generation.

Syn (Synergy): optics $\leftrightarrow$ transport coupling

$$\begin{aligned}
\text{(Optics)} \quad & A_{\text{base}}(\lambda; t, n, k) \xrightarrow{\text{fields}} G(x, \lambda), \\
\text{(Transport)} \quad & (\mu_{n,p}, \tau_{n,p}, S_{\text{f}}, S_{\text{b}}) \xrightarrow{\text{PDD}} \mathcal{C}(\lambda), \\
\text{(Coupling)} \quad & J_{\text{sc}} = q \int \Phi(\lambda)\, A_{\text{base}}(\lambda)\, \mathcal{C}(\lambda)\, d\lambda.
\end{aligned}$$

Operator view: Syn is the bilinear composition sending optical absorptance and electrical collection into photocurrent.

Reg (Regression/Stability): effective recombination relaxation

We model passivation and bulk improvement as a relaxation of effective recombination channels:

$$\begin{aligned}
\tau_{\text{eff}}^{-1} &= \tau_{\text{bulk}}^{-1} + \frac{2S}{W}, \quad J_0 \propto \tau_{\text{eff}}^{-1}, \\
\Rightarrow \quad \Delta V_{oc} &\approx n_{\text{id}} V_T \ln\left(\frac{\tau'_{\text{eff}}}{\tau_{\text{eff}}}\right).
\end{aligned}$$

Operator view: Reg maps $(S_{\text{f}}, S_{\text{b}}, \tau_{n,p}, \mu_{n,p})$ to a more stable (lower J_0) junction.

Cyc (Cyclicity): spectral/optical periodic structure

Two uses:

1. **Quarter-wave structure:** $t \approx \lambda_0/(4n_{\rm eff})$ exploits periodicity in optical phase $\delta \mapsto \delta + 2\pi$ to land near a benign reflectance valley.
2. **Spectral conditioning (optional):** projector on band-edge bands, e.g. $\mathsf{Cyc}_{[\lambda_1,\lambda_2]}[f] = \mathbf{1}_{[\lambda_1,\lambda_2]}(\lambda)f(\lambda)$.

Rec (Recursion): fixed-point tuning loop (conceptual)

If we iterate the coin to hit a target (e.g. maximize η subject to constraints),

$$\boldsymbol{c}_{k+1} = \mathsf{Rec}[\boldsymbol{c}_k] \equiv \Pi_{\mathcal{C}}\Big(\boldsymbol{c}_k + \alpha\, \Phi'\big(\boldsymbol{c}_k;\ \eta(\mathsf{State}(\boldsymbol{c}_k))\big)\Big),$$

with $\Pi_{\mathcal{C}}$ a projection onto physically admissible controls and Φ' any ascent direction.

Out (Outliers): moderated impulses in control space

$$\mathsf{Out}[\boldsymbol{c}]:\ \text{clip/floor } \{\gamma_k,\ t,\ S_{\rm f}, S_{\rm b},\ \tau_{n,p},\ \mu_{n,p}\}$$

to admissible intervals (e.g. $\gamma_k \ge 0$, $t \in [70, 110]$ nm for $k \approx 0$, $S_{\rm f} \in [80, 300]$ cm/s, $\tau \in [20, 50]$ ns).

Composite view

$$\underbrace{\mathsf{Comp}}_{\mathsf{Cyc}\circ\mathsf{Rec}\circ\mathsf{Frac}\circ\mathsf{Reg}\circ\mathsf{Syn}\circ\mathsf{Ref}\circ\mathsf{Out}} : \boldsymbol{c} \longmapsto \mathsf{State}(\boldsymbol{c}) \longmapsto \boldsymbol{r}(\mathsf{State})$$

with the concrete evaluation order during one forward solve:

$$\boldsymbol{c} \xrightarrow{\mathsf{Out}} \boldsymbol{c}^{\rm clipped} \xrightarrow{\mathsf{Frac}} k_{\rm eff}(\lambda) \xrightarrow{\mathsf{Ref}} \text{stack}(t, n, k) \xrightarrow{\mathsf{Cyc}} \text{phase-conditioned } t \xrightarrow{\mathsf{Syn}} (J_{\rm sc}, \text{QE}) \xrightarrow{\mathsf{Reg}} (J_0, V_{oc}, \text{FF}) \rightsquigarrow \eta.$$

13 What not to expect (without $n(\lambda)$ control)

- Big $J_{\rm sc}$ boosts from a single front layer are unlikely unless $n(\lambda)$ is tuned as a true AR layer or multi-layer stack.
- With $k(\lambda)$ taps only, $\gamma_k > 0$ always risks $J_{\rm sc}$ loss; the best optical policy here was $\gamma_k = 0$ and careful t.

Appendix: Units & conversions

- $\Phi(\lambda)$ from Solcore may be returned per nm: convert as needed; power density $P_{\rm in} = \int E_\gamma(\lambda)\Phi(\lambda)\, d\lambda$, with $E_\gamma(\lambda) = hc/\lambda$.
- Mobilities: $\text{cm}^2/(\text{V s}) \leftrightarrow \text{m}^2/(\text{V s})$ via $1\,\text{cm}^2/(\text{V s}) = 10^{-4}\,\text{m}^2/(\text{V s})$.
- Doping: $\text{cm}^{-3} \leftrightarrow \text{m}^{-3}$ via $1\,\text{cm}^{-3} = 10^6\,\text{m}^{-3}$.