Simplified Analysis of Internal Quantum Efficiency using Machine Learning

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Spectral analysis of internal quantum efficiency (IQE) measurements of solar cells is a powerful method to identify performance-limiting mechanisms in photovoltaic devices.[1] This analysis is usually performed using complex curve-fitting methods to extract various electrical and optical performance parameters.[1–3] Because these traditional fitting methods are not easy to use and often sensitive to measurement noise,[1–3] many users do not utilise the full potential of the IQE measurements to provide the key properties of their solar cells. In this study, we aim to simplify the analysis of IQE measurements of silicon (Si) solar cells using machine learning (ML). Powerful ML algorithms are trained to extract valuable information regarding the cell's performance, capable of replacing the traditional curve fitting methods.

IQE measurements indicate the ratio between the *collected carriers* and the number of *absorbed photons* by the sample.[1,4] It involves measuring the short circuit current, reflectance, and incident photon flux under variable monochromatic illumination.[4] Comparing the measurement results to the desired quantum efficiency of unity provides key information regarding the performance-limiting mechanisms of the device to photons of different energies.[1,4]

Traditional analysis methods of Si solar cells require fitting specific sections of the measured IQE to complex formulas.[1] An example is plotting the inverse IQE versus the wavelength-dependent absorption depth in Si. The inversed slope of this plot yields the effective diffusion length (L_{eff}) of the minority carriers in the base of the device.[1] This particular approach is usually limited to the near-infrared wavelength range and the resulting L_{eff} is strongly impacted by the selected wavelength range and measurement noise.[1,5] Other quantitative analysis methods involve mathematical models that are used to fit the measured IQE curve.[2,3,6] They often require manipulation of many parameters within the mathematical models, which can be time-consuming and complex depending on the number of unknown device parameters.[2,3,6]

The proposed ML-based framework aims to analyse IQE measurements automatically. It consists of training an array of random forest (RF) regressors[7] on a dataset of simulated IQE curves. The simulated dataset were constructed using the simplified integral formulas adapted from Fischer,[8] defined as:

$$IQE = X_{EMI} \times \int \eta(z) G(z) \cdot dz\,, \tag{1}$$

where X_{EMI} is the carrier collector term, while the bulk term is the integral of the bulk collection efficiency, $\eta(z)$, multiplied by the normalised generation profile, $G(z)$, over the cell thickness, z. The key independent parameters of X_{EMI} are the width of the emitter (w_e) and the emitter collection efficiency (IQE_0), while $\eta(z)$ is determined by the rear surface recombination velocity (SRV_b) and bulk lifetime (τ_b). The internal reflectance of the rear (RB) and the level of how diffuse light is after rear internal reflection (Λ) impact $G(z)$.

Different combinations of these six parameters were used to generate a dataset of 528,000 labelled IQE curves. The RF models were then trained on this dataset to extract the parameters from a given IQE measurement. Each RF model was trained to predict a single device parameter, forming an array of regression models. Hence, the proposed approach automatically decouples the front, bulk, and rear regions of an IQE measurement and provides the user with a compact list of the key electrical and optical parameters of the investigated device.[9]

The dataset was split into training and test subsets in a 70:30 ratio.[10] The test set results were evaluated using the root mean square relative error (RMSRE):[11]

$$\mathrm{RMSRE}(\boldsymbol{y}, \hat{\boldsymbol{y}}) = \sqrt{\frac{1}{N}\sum\nolimits_{i=1}^{N}\left(\frac{y_i - \hat{y}_i}{y_{max}}\right)^2}, \quad (2)$$

where $\hat{y}_i$ is the predicted value of the i^{th} sample, and y_i is the corresponding true value out of a total N samples. The relative error is calculated by dividing the absolute error by the maximum value in the parameter dataset, y_{max}. This metric was used to allow the prediction performance across different parameters to be easily compared.

Figure 1 presents the results obtained on the unseen test set, comparing the predicted labels with the true labels. The proposed RF-based method is capable of correctly predicting the emitter parameters (IQE_0 and w_e) as well as RB with negligible error. However, at this early stage, the regression models have larger errors in predicting τ_b and SRV_b, and fewer errors in predicting Λ. This occurs as there are multiple combinations of these three parameters that produce non-unique IQE points in the long wavelength range.

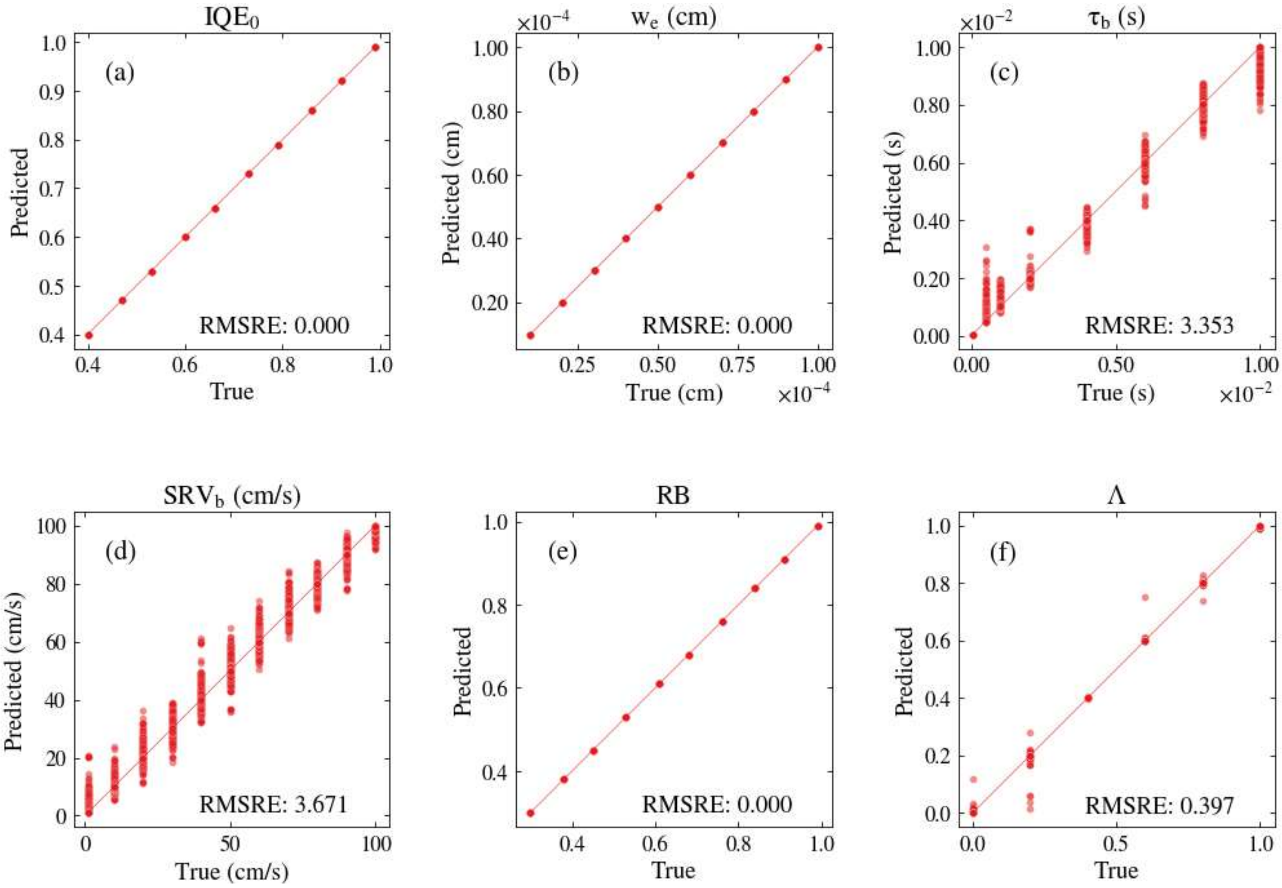
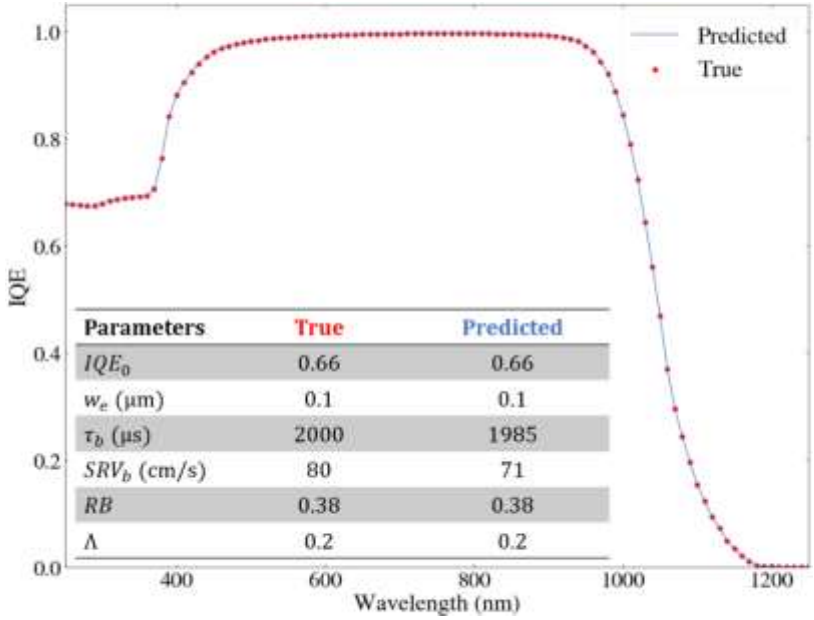


Figure 1 - Predicted versus true values for: (a) IQE_0, (b) w_e, (c) τ_b, (d) SRV_b, (e) RB, and (f) Λ. The RMSRE values are provided, where a higher value corresponds to higher prediction error.

Figure 2 compares the predicted and simulated ('true') IQE curves, i.e. the IQE generated using the input parameters vs the IQE generated using the parameters predicted by the ML-based approach. It can be seen that the ML model perfectly predicts most of the electrical and optical parameters, with errors in τ_b and SRV_b. As discussed above, this is an expected result due to the existence of non-unique IQE curves in the dataset. Nevertheless, these results provide a clear demonstration of the capabilities of the proposed method. Future work will involve improving prediction accuracy as well as extending the prediction capabilities to include the thickness and absorption profile of the front dielectric layer.



Parameters	True	Predicted
IQE_0	0.66	0.66
w_e (µm)	0.1	0.1
τ_b (µs)	2000	1985
SRV_b (cm/s)	80	71
RB	0.38	0.38
Λ	0.2	0.2

Figure 2 – Predicted and simulated IQE curves of a representative cell, generated from parameters listed in the inset table

To summarise, automated analysis of IQE measurements of Si solar cells using ML is presented and demonstrated to be a fast and simple method to extract key performance parameters of PV devices. By training ML models on a large dataset of simulated IQE curves, this study provides an accurate tool that is easier to use than traditional spectral response analysis methods. This method will be tested on experimental data in the near future and the results will be reported at the conference.

Acknowledgements

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