Extracting Parasitic Absorption and Layer Thickness from Optical Measurements by Combining Simulation and Machine Learning Techniques

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Introduction

The parasitic absorption J_A in a solar cell's front-side anti-reflection coating is an important parameter to optimize PERC cells for highest conversion efficiencies. However, it cannot be directly measured by optical characterization techniques and is thus commonly neglected in an approximate loss analysis or estimated from internal quantum efficiency (IQE) measurements. We present a theory-guided machine learning framework which combines machine learning and a physical model to extract the J_A and thicknesses from optical measurements.

Goal: Determine current loss and thickness values from optical measurements with input of reflectance R and ellipsometry curves ρ_{real}, ρ_{imag}

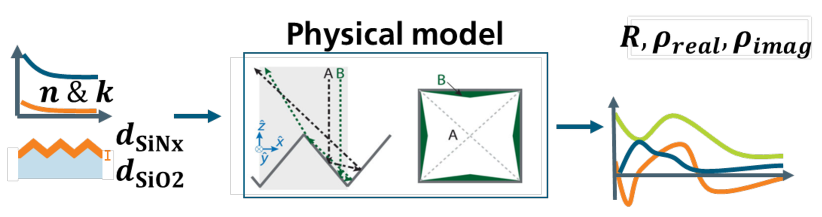
Challenges

- No reference information of J_A values for measurements available
  - Can be simulated with physical model for given optical parameters
  - Vice versa, optical parameters can be determined for given $R, \rho_{real}, \rho_{imag}$
- Numerical fitting is sensitive to initial parameters
- → Create and use synthetic data for machine learning
- → Design Self-supervised model which combines physics and machine learning and allows optimization with synthetic data and measurement data

Approach

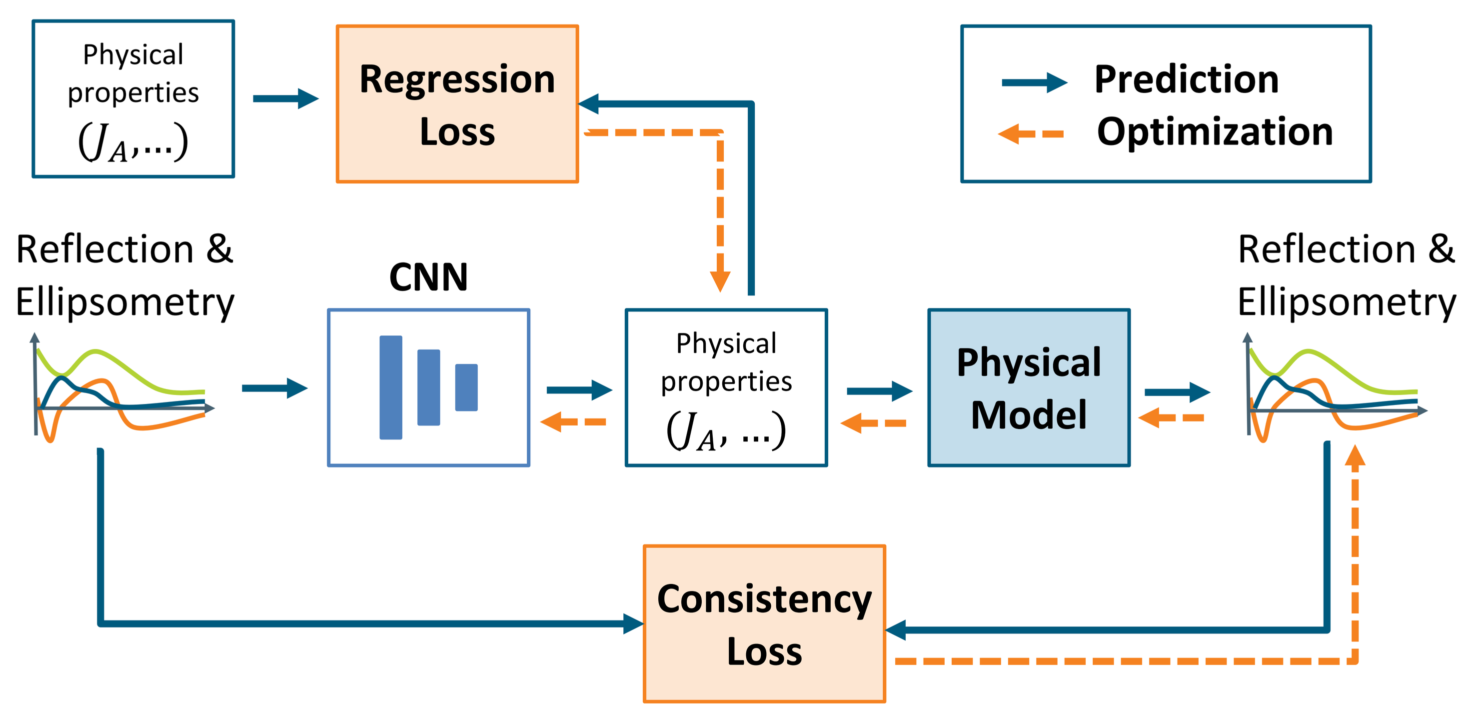
Physical model

- OPAL[1] Algorithm for reflectance and ellipsometry curve simulation
- Tauc-Lorentz approximation for refractive index simulation[2]



Hybrid model

- Convolutional neural network (CNN) determines physical properties based on reflection and ellipsometry data
- Subsequent physical model allows to reconstruct the input curves



- Optimization 1: By layer parameter and spectral curve comparison for synthetic data
- Optimization 2 (refinement): Solely self-supervised by curve comparison for measurement data (consistency check compares input and reconstruction)

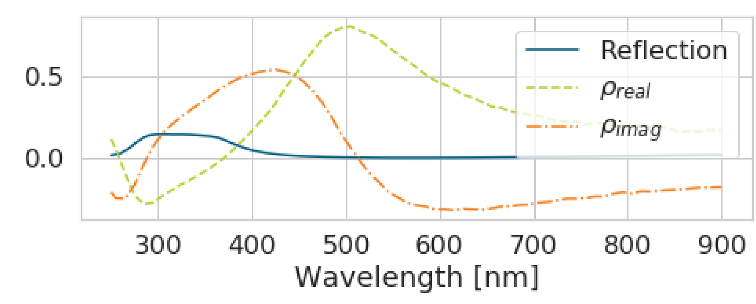
Training data

Dataset 1: Simulated data with realistic parameter range

- 40,000 samples simulated with refractive data from literature[3]
- Pairs of reflectance/ellipsometry curves together with optical parameters

Dataset 2: Measurements

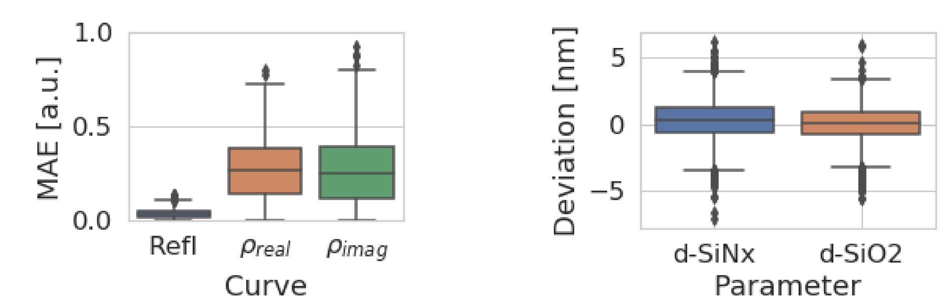
- 12 silicon wafers with textured surface and SiNx anti reflection coating
- 3 different manufacturers
- 4 wafer per group
- Spectrometer: 16 spots per wafer
- Ellipsometer: 1 spot per wafer

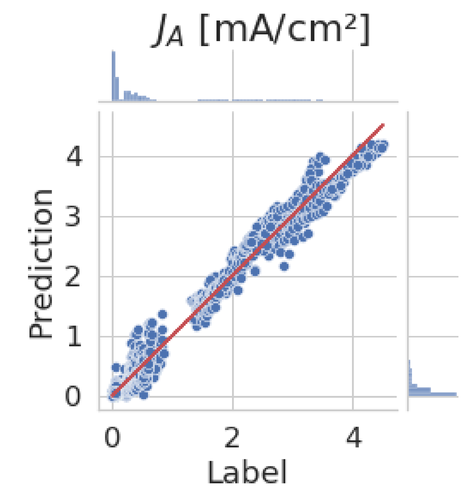


Results

Results on simulated data (dataset 1, 4000 test samples)

- Good correlation between known parameters and prediction
- Thickness prediction error for 90 % of all samples below 5 nm
- Mean average error (MAE) for J_A: 0.08 mA/cm²

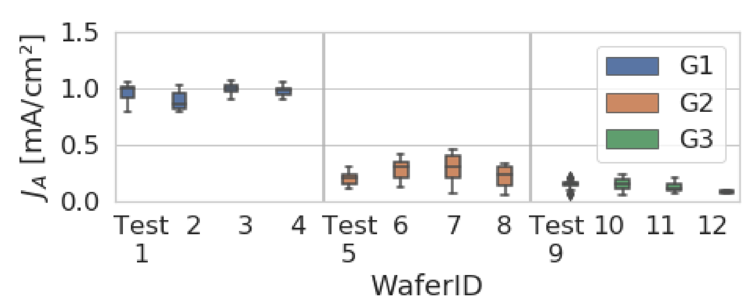




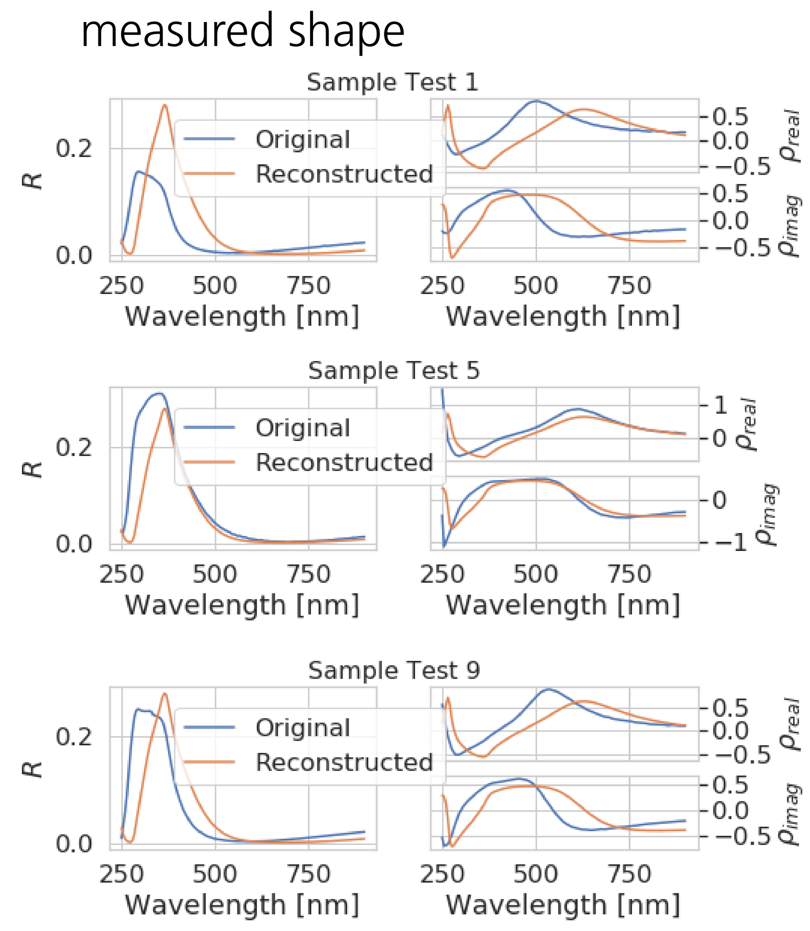
Results on measurements (dataset 2)

Optimization 1

- J_A value prediction consistent within each group

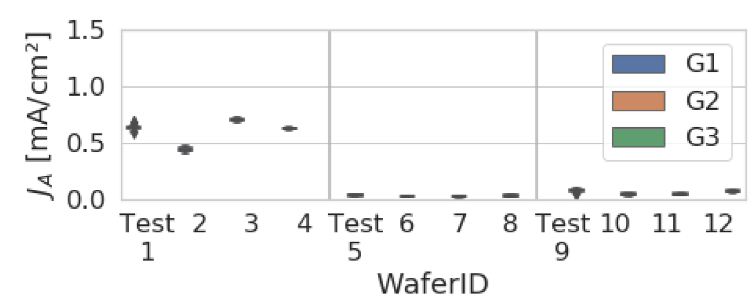


- Reconstructed curves follows the measured shape

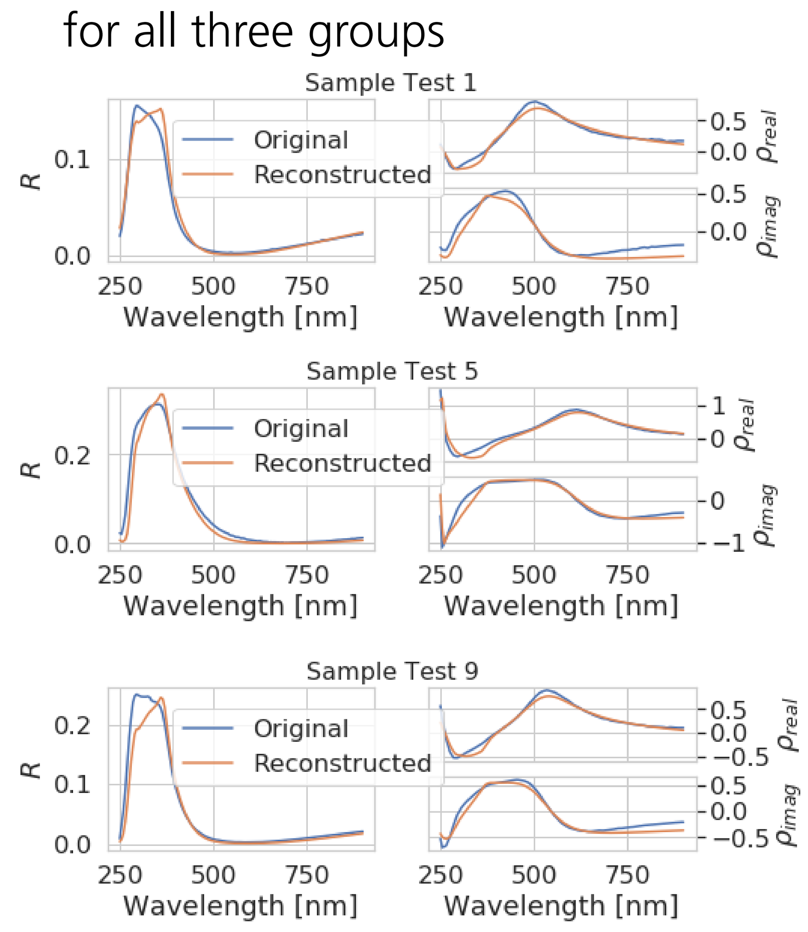


Optimization 2 (Refinement)

- Training with 3 samples per group, 1 sample for evaluation (16 spots)



- Improvement in curve reconstruction for all three groups



Next step: validate parameter prediction with reference characterization

Summary

- J_A determination works well on simulated data
- Hybrid model provides physically interpretable results
- Consistency check allows training on measurements even without labels for physical parameter
- Finetuning with consistency check improves curve reconstruction

[1] Baker-Finch et al., PIP, 19(4), 2011
[2] Rodríguez-de Marcos et al., Opt. Express, OE 24 (2016)
[3] www.pvlighthouse.com and internal measurements

Link to Fraunhofer ISE contributions of the 40th EU PVSEC https://ise.link/eupvsec2023 (available as of 20.09.2023)

This work was funded by the German Federal Ministry for Economic Affairs and Climate Action within the project KISS PV (020E-100485635)