MSc project: Efficient optimization algorithms for efficient solar cells

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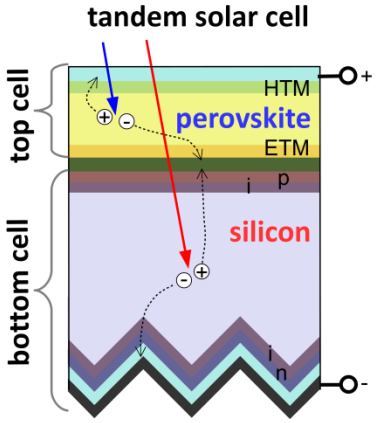
Solar cells are multi-layered structures that absorb incoming sunlight and transport the thereby mobilised positive and negative charge carriers to the contacts. Today the next generation of solar cells is being developed, so-called perovskite / silicon tandem (double junction) solar cells, that can achieve a higher power conversion efficiency than the conventional (single junction) silicon solar cells that dominate the market today [1]. Researchers use physical models to predict the efficiency of these tandem solar cells. The most important input parameters are the material and thickness used for each layer. Using these models, calculating solar cell efficiency takes several minutes of computing time.



As shown in the figure above, tandem solar cells consist of a silicon substrate, with a standard thickness of 200 um, on which about 10 layers, with thicknesses between 5 and 500 nm, are deposited. The optimum solar cells design consist of the combination of layer thicknesses that gives the maximum efficiency. Because the calculation of every possible thickness combination in this 10-dimensional parameter space would take too much computation time, optimization algorithms are required. **The goal of this project is to find the most efficient solar cell optimization algorithm.**

There are several requirements for the algorithm. Firstly the algorithm should not get stuck in a local optimum, but try to find the global optimum. Secondly, input parameters like layer thickness have minimum and maximum allowed values, which should be respected by the algorithm. Thirdly, the algorithm should be able to deal with a combination of *continuous* input variables, such as layer thickness, and *discrete* input variables, such as layer material. For example, the algorithm should be able to determine the most suitable electron transporting material from a list of available materials. Fourthly, the algorithm should be able to deal with an inherent error margin in the objective function, i.e. the calculated efficiency. This is because the physical models for calculating the efficiency are based on Monte Carlo methods and therefore do not yield exactly the same efficiency when rerunning the model again with the same input parameters.

A wide range of optimization algorithms exist, such as simplex search method, interior-reflective Newton method, genetic algorithm, simulated annealing, etc. , each with their strengths and weaknesses. Some of these algorithms can deal with the first and second requirements mentioned

above, but it is not known whether they can satisfy the third and fourth requirement. This means that existing optimization algorithms might need to be extended or combined in order to arrive at the most efficient optimization algorithm. Note that optimization algorithms have already been used for solar cell optimization [2-4]. This previous work should be studied as part of the literature review.

[1] Jérémy Werner, Bjoern Niesen and Christophe Ballif, *Perovskite / Silicon Tandem Solar Cells: Marriage of Convenience or True Love Story? – An Overview*, Advanced Materials Interfaces **5** (2018) 1700731. https://doi.org/10.1002/admi.201700731

[2] Ahmer A. B. Baloch, Shahzada P. Aly, Mohammad I. Hossain, Fedwa El-Mellouhi, Nouar Tabet and Fahhad H. Alharbi, *Full space device optimization for solar cells,* Scientific Reports **7** (2017). https://doi.org/10.1038/s41598-017-12158-0

[3] F. Pelanchon and P. Mialhe, *Optimization of solar cell performance,* Solid-State Electronics **33**(1) (1990). https://doi.org/10.1016/0038-1101(90)90008-3

[4] M. Hoogwerff, Optimization Algorithms for Improving the Efficiency of Tandem Solar Cells, BSc. Thesis, TU Delft (2020).