Machine Learning Assisted Material and Device Parameter Extraction From Measurements Of Thin Film Semiconductor Devices

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***Abstract*—The simulation of thin film semiconductor devices is challenging, partly due to the unknown material and device parameters. In this contribution, we present two different approaches to determine the missing material and device parameters from measurements. They both have in common that they are based on machine learning (ML) and numerical models. First, a numerical model describing the experiment is used to generate synthetic data to train a machine learning model the underlying material parameters. After successful training, a measurement is presented to the ML model to predict the parameters. In a more recent physics-informed ML approach, we integrate the model into the ML method and thus reduce the training data set.**

***Index Terms*—synthetic data, material parameter extraction, PINNs, thin film semiconductor device**

I. Introduction

To further improve organic light-emitting diodes [1] (OLEDs) and other optoelectronic devices in terms of e.g. stability and efficiency, a model describing all major physical processes in the optoelectronic device is of high importance. Such models rely on the availability of material parameters. These parameters are usually obtained by tailored measurements. Nevertheless, they can vary for different measurement techniques, depend on the neighbouring layers, or are not accessible by measurements. In these cases, least-square algorithms where the the sum of squared differences between the measurement and simulation is minimized by varying the material parameters are used to determine the parameters. Depending on the number of parameters and their correlation the task may become quite complex and requires domain knowledge to guide the search in the right direction. With the rise of ML techniques in the last decade, we will try to combine the advantages of ML with the numerical model.

II. Data generation and ML training

In the first approach, we employ a numerical model to generate a synthetic data set that is then analyzed by a ML model as explained in more details in [2]. In Fig.1 the workflow to extract the material parameters is outlined.

In the example, seven material/device parameters of an organic single carrier p-doped/intrinsic/p-doped device [3] were randomly varied in a given range as found in literature [2], namely the work function, mobility, mobility field-enhancement factor (Poole-Frenkel mobility model), doping density, the relative permittivity of the intrinsic and doped material and the series resistance. For each parameter variation, a current-voltage curve and impedance spectroscopy simulation [4] were performed contributing to the final set of 100’000 variations. The set was then split into training data that is shown to the ML model [5], [6] for learning purposes and a test data set used for validation of the ML model on ”unseen” or new data. Once the performance on the test set is satisfying, the measurements [7] are evaluated by the ML model resulting in the underlying set of material parameters.

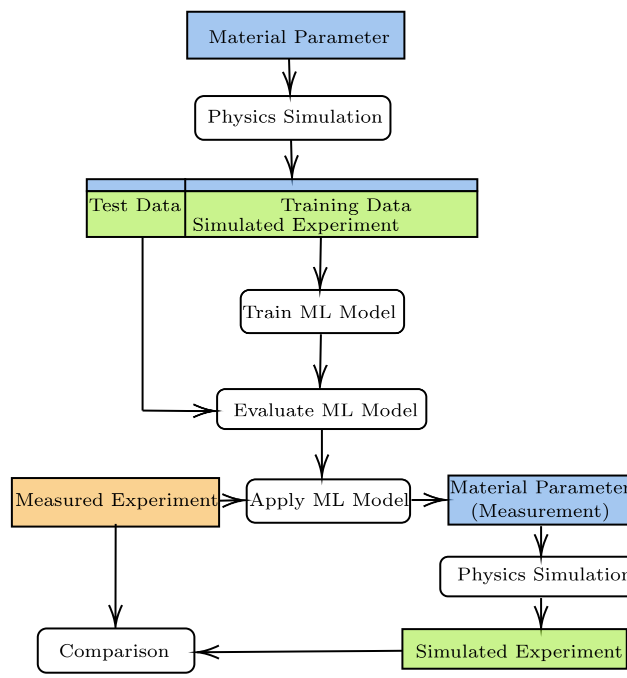

Fig. 1. Workflow of synthetic data generation and subsequent machine learning and validation on the measurement data according to [2].

In Fig. 2, we compare the fitted and measured experiments for three different device thicknesses. The parameters found are in agreement with the results of a traditional fitting approach [3]. To further improve the results, the parameter set could be used as a starting point for a traditional least-square fitting optimizer. The same procedure as described above was applied in [8] where we analyze the electroluminescence image of a silicon solar cell with the aid of a convolutional neural network and a 1+2D approach for the solar cell model.

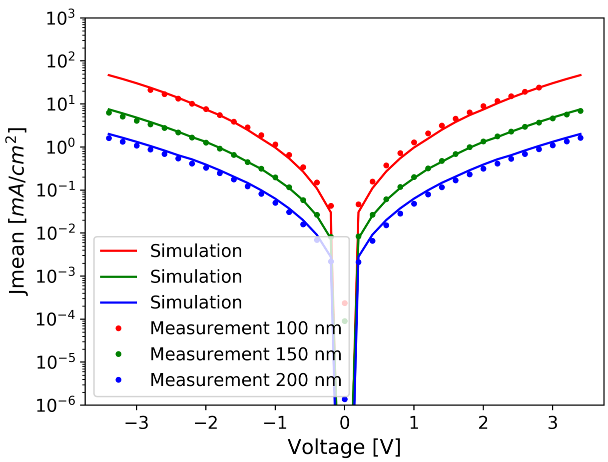

Fig. 2. The current-voltage curves for all three thicknesses are shown, additionally impedance measurements were also compared, for more details see [2].

III. Physics-informed ML

The disadvantage of the above approach is that we only profit form the physical knowledge in the numerical model to generate the data. In the second step, the ML model has to re-establish the underlying pattern. In order to enable successful learning, a big enough data set is required resulting in a huge amount of simulations and considerable computational time. Thus, it would be desirable to integrate the physical knowledge more directly. In physics-informed neural networks (PINNs) [9], [10], the PDEs describing the model are built into the loss function of the neural network. In the case of the parameter extraction problem, we minimize a loss function consisting of the norm of the difference of the measurements and the neural network solution and the PDEs' residuum of the neural network solution. The total amount of parameters to be determined consists of the weights and biases of the neural network and the material parameters. After successful training of the PINN, the PDEs are fulfilled and the material parameters found. The training of the neural network, however, can be challenging and is subject of current research [9], [11]. The advantage of PINNs is that they seamlessly integrate the measurement data and we profit from automatic differentiation as well as the strengths of deep neural networks and frameworks [12]–[14].

IV. Conclusion

The extraction of material parameters from measurements is crucial for device optimization and remains challenging. Besides conventional fitting approaches, new methods from the machine learning field are emerging and expanding into physical modelling. We presented an approach where the numerical model is used for synthetic data generation and parameters extraced by ML. The amount of data is reduced by combining the model with the ML method leading to the second appraoch known as PINNs. They integrate seamlessly noisy data and take advantage of the deep learning infrastructure.

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