Degradation Lifetime Modeling for Perovskite Photovoltaic Modules

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***Abstract*—We describe a workflow for the lifetime simulation of Perovskite solar modules, that combines modeling of water ingress and of the resulting local effects due to humidity with simulation of the cell stack, possibly including other degradation channels like defect formation, and with a lumped element SPICE model of the solar module. Such a model would allow to predict module performance throughout module lifetime. Here we present in particular an initial implementation of water ingress simulation linked to the lumped element module model.**

***Index Terms*—Photovoltaics, Perovskite, solar module, water ingress, simulation**

I. Introduction

Since their first appearance, metal halide Perovskite based solar cells have by now reached record efficiencies of 26.95% for single junctions and 34.6% for Perovskite/Silicon tandems [1]. One of the main issues impeding large scale deployment and thus still to be resolved is related to long-term stability of Perovskite-based cells. Although progress has been made, device stability and degradation is an active area of research. Presence of moisture is known to be of major importance in Perovskite material degradation [2], [3]. Therefore, proper encapsulation of Perovskite modules is a critical step in slowing down ingress of moisture into the active material. In addition, carrier-injection induced formation of point defects can be an issue in halide Perovskites [4], which could result in reversible or irreversible and possibly mobile ionic defects, inducing additional time-dependent performance variation.

II. Proposed simulation model

We propose a composite model linking the following three submodels, illustrated in Fig. 1. The first model describes water ingress into the module, based on Fick's law, driven by the water vapour pressure in the atmosphere surrounding the module [5]. The problem is described by the parabolic partial differential equation

$$\frac{\partial Sp}{\partial t} = \nabla \left(D \nabla Sp \right) \text{ on } \Omega, \; p = Sp_0 \text{ on } \partial\Omega, \qquad (1)$$

where p is the water vapour partial pressure, S is the solubility, D is the diffusivity, and Ω is the simulation domain including the encapsulation. The water concentration is given by $c = Sp$. We assume the module to be encapsulated between two glass sheets, so that a 2D approximation with lateral ingress is justified.

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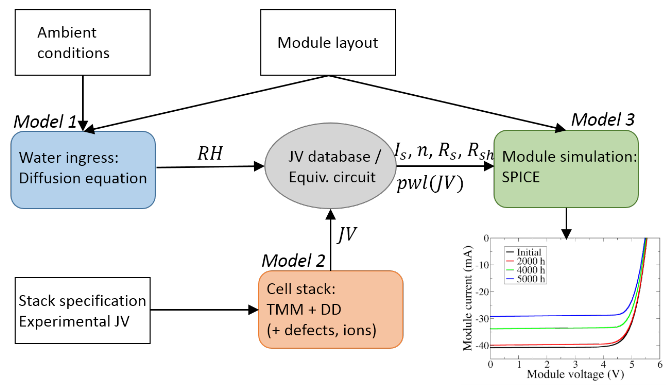

Fig. 1. Simplified scheme of the modeling approach, highlighting the three linked simulation models and their connections.

The second model describes the cell stack, and provides locally the current-voltage characteristic in a 1D approximation. Here, a drift-diffusion model could be used to create a dataset of device characteristics under different operating conditions (degradation state, illumination, defect formation, etc.), in order to form a parameterized dataset for the third model. At this stage, fitting to experimental data on degraded research cells could be useful.

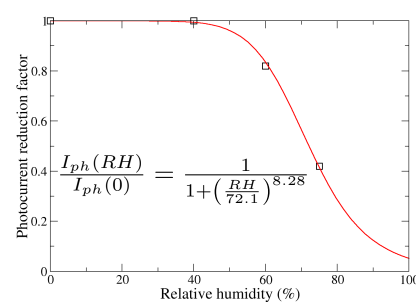

Fig. 2. Reduction factor for short circuit current, fitted to the data (symbols) extracted from [3].

The third model uses an electronic circuit approximation of the module in terms of concentrated elements, using SPICE to solve the circuit model [6]. The 2D module layout is descritized into finite patches, and to each patch an elementary

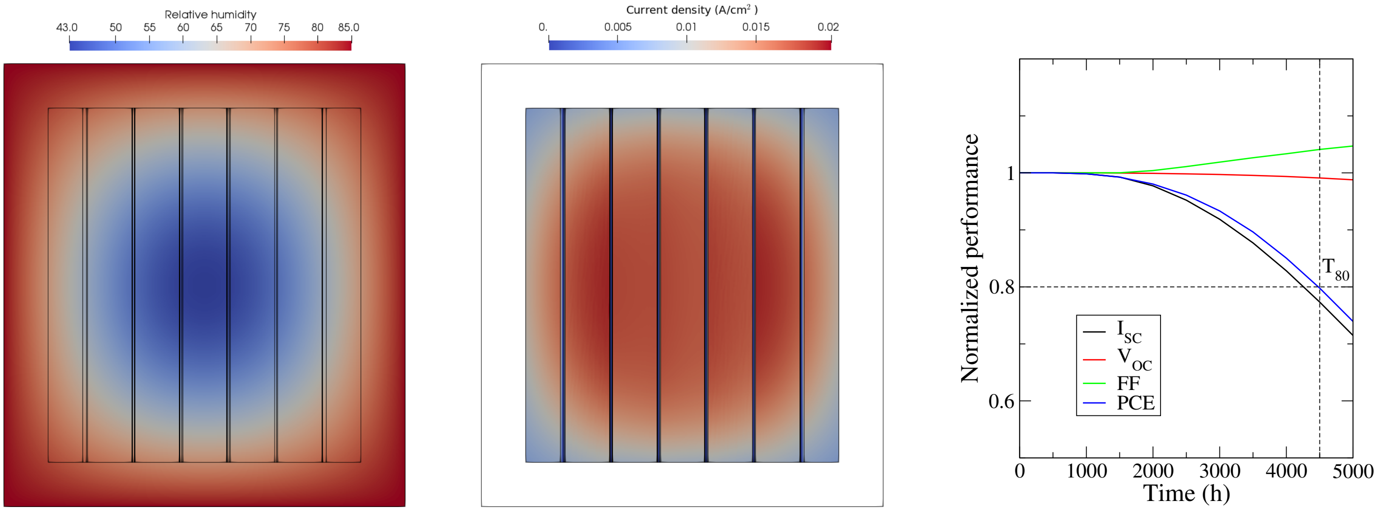

Fig. 3. Relative humidity in the module (left), and local current density across the elementary cells (middle), after 4500 h in 85% humidity and room temperature. On the right the time evolution of the normalized module performance parameters. The fill factor (FF) increases slightly, because the model used here only results in a reduction of the short circuit current, while open circuit voltage (V_{OC}) remains almost unchanged. At $T_{80} \approx$ 4500 h, the PCE reaches 80% of it's initial value.

cell stack is assigned, while different cells are connected on the top and bottom layers via lumped resistors, obtained from the contact layer sheet resistivities. The elementary cell can be described via its numeric JV characteristic, using a piecewise-linear voltage controlled source (pwl), or via an equivalent circuit. In both cases, the data from the cell stack model can be used to obtain a SPICE model parameterized in terms of relevant quantities such as relative humidity, temperature, light intensity etc. The connecting resistors are obtained from a 2D finite element or finite volume discretization of a steady-state diffusion equation. The implementation allows thus for unstructured discretizations of the module geometry, increasing versatility. All models are implemented in tibercad software [7], while for the SPICE engine we used ngspice [8]

III. Preliminary results

We have performed a preliminary simulation of a 10.96 cm^2 minimodule with five $4{\times}0.5$ cm^2 subcells in series, assuming an additional 5 mm lateral sealing. For the water ingress simulation we used parameters of EVA, i.e. diffusivity $D = 3.43 \times 10^{-11}$ m^2/s and solubility $S = 0.45$ g/m^{3}Pa [5]. For sake of simplicity, we did not consider water diffusion in the perovskite itself, leading to an overestimation of the lifetime. Data on reduction of absorption in a Perovskite cell as a function of relative humidity has been taken from [3], and fitted to a humidity-dependent model of the short circuit current density as shown in Fig. 2. A measured JV characteristic of a research cell has been used to fit a one-diode equivalent circuit, that has been used as elementary cell for the SPICE model. For the water ingress simulation, we assumed a boundary condition of 85% relative humidity at 300 K. The water diffusion model has then been solved until 5000 h, and every 500 h the module model has been solved, using the relative humidity in every cell to modify the I_{SC}. Figure 3 shows the spatial distribution of relative humidity in the module after 4500 h, the resulting vertical current density through the elementary cells, and the time evolution of the module performance. For the used parameters and geometry, a T_{80} of approx. 4500 h is obtained.

The initial implementation presented here will be further extended. In particular, the elementary cell equivalent circuit will be generalized to 2- and 3-diode models, and an alternative definition of the elementary cell patches based on the primal mesh elements will be implemented. Also, the model needs to be tested under realistic conditions.

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