MODELLING INFRASTRUCTURE ALONG THE VALUE CHAIN: FROM MATERIALS TO SYSTEM PERFORMANCE

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ABSTRACT: This paper reports on progress towards the development of an infrastructure to integrate existing modelling tools, and thus allow modelling of the entire solar cell value chain, from initial material parameters to the long-term energy yield of complete PV systems. Currently, the infrastructure has been developed and successfully tested from the material to the system level, for three different cell technologies using 13 different programs across 7 European institutes. Input data can be either modelled or experimentally measured. Further work will focus on: comparison of the simulation results with experimentally measured system data; defining standard interface protocols to simplify the information transfer; and predicting the yearly energy output for installed PV systems.

Keywords: modelling, a-Si:H, CIGS, heterojunction, system, system performance

1 INTRODUCTION

There are a large number of software programs currently available to simulate various solar cell technologies at processing stages from material modelling through to complete systems. The current problem is that although the modelling expertise for each of these stages exists, it is widely scattered across Europe.

Within the European project SOPHIA we are developing an infrastructure, which will allow these scattered modelling tools and expertise to be combined into a full value chain modelling approach. The final vision is an interactive toolbox of existing or new modelling software, from which specific tools can be selected and merged into a full-scale modelling approach. One of the key challenges that must be overcome is the development of a standardised interfacing between all models.

In the following sections, we report on the details and progress towards the development of such a toolbox. We demonstrate a working chain for each of a-Si, CIGS, and Si-Heterojunction cell technologies, and provide the final simulated system performance. An overview of some available models and necessary interfaces is described in section 2. The chain from material to module modelling is discussed for each of these technologies in sections 3.1 to 3.3 respectively, and the module-system interaction and system output are described and discussed in section 3.4.

2 METHOD / OVERVIEW

The value chain and specific interfaces between modelling tools are exhibited in Figure 1. In the figure, the materials to be modelled are listed. At all other modelling levels, commercially available modelling tools are designated by the software name, and in-house designed tools are designated by the research institution.

![Figure 1: Overview of available institutes and models (blue squares), and necessary interfaces. The black squares show the required device data for interfacing, and the red boxes contain the environmental input parameters. The three chains discussed in this paper are shown: silicon-heterojunction in blue, a-Si:H in yellow, and CIGS in green.](image)

The overall structure of the interface is simple. There are four levels of simulations in the chain: atomic level material simulations, solar cells, modules, and complete systems. The system simulation output can then be used to predict the yearly energy output of specific PV systems based on detailed physical models. The input data for each level can either be simulated or experimentally measured, depending which parameters will be varied in each level of the model.
3 RESULTS

3.1 Amorphous silicon (a-Si) technology

Amorphous silicon was chosen as the first test case for the material modelling and the material-cell interface. The material modelling was performed at ENEA. Amorphous silicon material was simulated by atomic-scale ab-initio calculations, using the CPMD (Car-Parrinello Molecular Dynamics) and QE (Quantum Expresso) numerical codes. Interfaces were characterized in terms of atomic bonding and chemical interactions. The contribution of defects was fully taken into account. These atomic scale systems were modelled using high-performance parallel computing platforms available in the Sophia infrastructure.

The modelling input is the number and type of atoms. The output of the CPMD simulations is the evolution in time of both the atomic coordinates and the electronic structure, which leads to a final physical and electronic structure of the material. Currently, the material modelling has successfully simulated a-Si in an equilibrium state, as defined by the generation and recombination of dangling bonds. Several macroscopic physical quantities, such as the absorption coefficient and the energy distribution of defects were computed from the equilibrium simulation output. These have been correlated with macroscopic physical quantities.

Those macroscopic quantities calculated from the material modelling output have been used as input for cell simulations. However, the modelling of “real” (non-equilibrium) device relevant a-Si structures and the extraction of further macroscopic properties as input for cell modelling are still in discussion.

The material to cell interface is the most difficult of all interfaces to standardise, as it requires knowledge of how to calculate relevant macroscopic material parameters from the atomic coordinates and electronic structure.

Due to the complexity of this interface for a-Si, we will not aim to standardise the interface and implement it in a database in SOPHIA. Instead, we will use the internal and external collaboration to make current a-Si models more scientifically rigorous.

Modelling of amorphous silicon solar cells was successfully performed at Jülich using optical data input into the electrical simulation software ASA [1]. To model the I-V curves required for the cell-module interface, an a-Si solar cell with a stabilised efficiency of 9.9% was characterised in its stabilised state with temperature dependent light and dark I-V curves and differential spectral response. These data were input into ASA, and used to calibrate the model data for one-sun irradiation and a temperature range of 15°C-65°C. ASA was then used to calculate the cell I-V curves for the significantly larger temperature and irradiation range required for the system modelling.

The module I-V curves were calculated at Jülich, taking in the cell I-V curves, cell length, width, sheet resistance, parallel resistance, and the number of cells in the module. The series resistance is calculated using a first order approximation. Each cell is assumed to have one perfect conducting electrode, and one resistive electrode. The cells are assumed to have a uniform diode current and the bias voltage is assumed to be the average cell voltage. The module I-V curves are then output for the temperature and irradiation range required for system modelling.

3.2 Cu(InGa)Se2 (CIGS) technology

As can be seen from Figure 2, a number of different programs have been successfully interfaced in the CIGS chain. Two different material compositions of CIGS cells were modelled. These were used to model a module of uniform quality cells (as required for the system model), as well as the influence of a single defected cell on a CIGS module. Both modules were compared.

The complex refractive index (n and k) was derived for CIGS films with two different Ga ratios (0.33 and 0.77), using the RefDex program developed in-house at HZB. RefDex is based on the theory of the Transfer-Matrix method. It accounts for surface roughness, and extracts n and k from measured transmission and reflection. [2]

These optical constants were input into the Sentaurus TCAD simulation program at TU Berlin, which included a Shockley-Read-Hall recombination model for the electrical simulations. The Sentaurus program calculated the optical generation in the CIGS cell, and output the dark and illuminated cell I-V characteristics. Series and shunt resistances were not included. TU Berlin also supplied data for two Ga concentrations and the layer thickness. Effective diode parameters were calculated from this data, and the photogenerated current density was assumed to be equal to Jsc. Using this output data, a four-cell module with monolithic interconnect was simulated, using two different simulation tools.

The first method, at ECN, used an in-house developed program to solve a set of coupled Poisson equations using the Finite Element Method (FEM) [3,4]. The cells are described by a set of parallel equivalent one-diode circuits. Each cell consists of an active layer and two contact layers with non-zero resistivity. Input parameters are equivalent circuit parameters taken from fitting of the cell I-V curves (Jsc, J0, ideality factor and Rshunt), layer thickness and conductivity, cell geometry, and defect position. The spatial resolution of the model is between 2000 and 4000 equivalent circuits per cell. Variations in shunt resistance and scribe width were modelled. In addition, calculations were done with two local areas of poor diode characteristics (high dark saturation current density) in the module. Calculation time is 20s per I-V point for each cell. The model can output module I-V curves, 2D plots of current density and voltage, and the location and distribution of power dissipated within the module.

The second method used the program NGSpice to perform a 2D electrical circuit simulation. An in-house program was developed at Jülich, which used the cell data output by TU Berlin, as well as defined module properties to calculate the input file for NGSpice. The results published in [5] show extremely good agreement with an experimentally measured DLIT image.
In order to test the cell-module-system chain, standard CIGS cells as described in [6] were modelled at TU Berlin, using the SCAPS program [7]. Cell I-V curves for temperature and illumination range required for the system model were output. These I-V curves were then fitted with a one-diode fit using Origin, and the cell parameters required for the module model (Jsc, J0 and the ideality factor n) were extracted. The module modelling was done at ECN, using the previously described program.

The results of the CIGS system modelling are presented in section 3.4.

3.3 Silicon heterojunction

The silicon heterojunction chain is represented in figure 1. Solar cells were simulated at INES-CEA, using the commercial simulation software Silvaco Atlas. 2D structures were implemented, incorporating the complete stack of state-of-the-art cells: standard high quality 150 µm thick (n)c-Si wafer (resistivity=3 Ohm cm), (i)a-Si:H buffer layers on both sides, (p)a-Si:H emitter layer on the front and (n)a-Si:H back surface field. The a-Si:H stacks are covered by a TCO. Contacts are assumed to be ideal and infinitely thin on both sides. Interface and bulk defects in a-Si:H layers were taken into account. A pseudo-texturization allows simulation of current values close to values expected from experiments. The temperature variation is taken into account for the bulk (temperature dependent Fermi-Dirac and Shockley-Read-Hall statistics) as well as at the interfaces (thermionic emission transport). Band offsets were varied according to [8]. Cell I-V curves were calculated for the temperature and irradiation range required for system modelling.

Approximate Si-heterojunction module I-V curves were calculated using the following method. Module data was obtained from the Sanyo HIT cell data sheet [9]. Module series resistance was extracted from the data using a method similar to that described in [10]. This resistance was converted to a resistance per cell and compared to the series resistance of the simulated cells. The difference was assumed to be the module interconnection resistance. This value was incorporated into the Silvaco-output cell I-V curves, by calculating the voltage including the series resistance using $V_{th} = V + IR_s$. The modules were simulated as 72 (12.7cm x 12.7cm) cells in series.

3.4 System modelling

Complete systems of all three cell technologies were modelled using a program developed in-house at Fraunhofer ISE. The PV system model has been described in detail in [11]. It combines the simulation of the irradiance by ray-tracing with a detailed temperature simulation approach and calculates the system I-V curve for every time step, combining the I-V curves of every PV cell. The model ideally requires an input data set of approximately 25000 module I-V curves, calculated for the required temperature and irradiation range. For 1D cell and module simulation programs, this is not an unreasonable request, as such a data set can be calculated in a matter of hours. However, for 2D and 3D programs, where each I-V curve can take minutes to simulate, this data set requires an extremely large amount of computing time. In these cases, the data set required from the module modelling programs was reduced by increasing the step size within the irradiation and temperature ranges. The output data was then interpolated to get the step size required for input into the system simulation.

The simulations are performed based on a meteorological data set, consisting of two irradiance values (in most cases the global-horizontal and the diffuse-horizontal irradiance) and the ambient temperature for each time step. The sky radiation distribution is calculated from the irradiance values, and then a ray-tracing procedure is used to calculate the irradiance on every PV cell of the system, as a function of time.

The model can take complicated shading or irradiation patterns and temperature variations into account. These patterns can be specified down to the level of individual cells, and include the effect of the installed bypass diodes. However, for simplicity, the effects of shading and temperature variations were not included in the work in this paper.

The last element of the system model is the inverter. In this case, an SMA 3000HF inverter was specified for all three PV systems. The inverter specifications, such as the limitation of the MPP voltage range and the constant voltage mode for low irradiance levels are taken into account, and the DC and AC values of the PV system over time are calculated. Finally, the inverter efficiency is calculated based on the DC power and the DC voltage. A complete, detailed description and validation of the model can again be found in [11].

For the simulations within this paper, the meteorological data from 2005 were used. The irradiance is calculated based on a PV system in Freiburg i.B., with a standard tilt angle of 30° and southern direction. The module temperatures are calculated assuming the PV system is a free-standing PV plant. The ground albedo is set to a standard value of 0.2, and the PV system is assumed to be homogeneously irradiated over the whole year.

Module and system parameters were chosen such that the same inverter could be used for all three PV system simulations. Geometrical and electrical module data, and final system configuration, are presented in Tables 1, 2, and 3 respectively.

Using these specifications, and the data input from the module modelling, the final output AC output energy for the the amorphous silicon, CIGS and Si-heterojunction PV systems was calculated to be 3492.0 kWh/year, 3756.8 kWh/year, and 3739.8 kWh/year respectively. It should be noted that material, cell and system properties were chosen for modelling convenience, and so comparison of the three PV technologies is not possible.
The project goal is to make the standard interface protocols available to all researchers that require it. The final vision would be a standardised method of accessing the chain, either by contracting and paying the relevant institutions, or by allowing either public or restricted access to the database and toolbox via a website.

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