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The concept of skins for silicon solar cell modeling

Andreas Fell[a,*], Jonas Schön[a], Martin C. Schubert[a], Stefan W. Glunz[a,b]

[a] Fraunhofer Institute for Solar Energy Systems (ISE), Heidenhofstrasse 2, 79110 Freiburg, Germany
[b] Department of Sustainable Systems Engineering, Albert Ludwig University of Freiburg, Georges-Köhler-Allee 103, D-79110 Freiburg, Germany

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ABSTRACT

Within (crystalline silicon) solar cell modeling, a skin means the *thin* region from the quasi-neutral bulk to the actual surface or metal contact, including e.g. doping profiles, induced band-bending or top-cells of a tandem configuration. A typical highly doped skin is commonly characterized by its main lumped properties: effective recombination via $J_{0,skin}$ and lateral conductance via R_{sheet}. When applied as a boundary condition to bulk carrier transport modeling, it is known as the conductive boundary model. However, the detailed resolution of physics inside the skin is then lacking but required in many cases, and possible complexities, like injection dependence of the lumped parameters, are commonly neglected. This work introduces a general parameterization of skins, which accounts fully for injection dependence and a vertical resistance, and is thus able to accurately describe arbitrarily complex skins by lumped parameters. A "skin solver" is implemented in the solar cell simulation software Quokka3 to solve a detailed skin in 1D and to perform the general parameterization. Additionally, the performance of the multidimensional quasi-neutral bulk (qn-bulk) solver is largely improved compared to Quokka2, enabling, for the first time, the 3D discretization and solution of up to an entire 156 mm × 156 mm solar cell in manageable computing times. Quokka3 can then consistently couple the skin solver with the qn-bulk solver. With this multiscale modeling approach, the user can define and solve a solar cell device including the details of the skins orders of magnitude faster compared to generic device simulation software, without loss of accuracy for the majority of conditions in wafer-based silicon solar cells. The new capabilities are demonstrated by showing how the front phosphorus diffusion of a PERC solar cell can be optimized with unprecedented completeness and accuracy. Besides accurately modeling 3D current transport in the bulk, the single solution domain intrinsically accounts for the busbar influence (both recombination and shading), the distributed resistance of the fingers, and the limited current collection independent of the surface area enlargement by texturing.

1. Introduction

When modeling crystalline silicon solar cells, three main regions of the device can be distinguished: a) the quasi-neutral and lowly doped bulk, which is relatively thick and acts as the main photon absorber, b) the skins [1], which are the thin near-surface regions selectively conducting electrons or holes to the metal contacts (laterally and vertically), and c) the metal grid. While current transport in the (quasi-neutral) bulk and the metal is relatively easy to model, the skins contain more challenging physics like for example high doping density with strong gradients, a space-charge region, induced band bending, multiple material layers etc.. It is therefore popular to describe a skin by its lumped properties, typically by an effective recombination property $J_{0,skin}$, and sheet resistance R_{sheet}. Those lumped properties, which are usually well measurable, can be used as a boundary condition when solving bulk carrier transport, greatly simplifying the modeling and thus enhancing speed for numerical solvers [2]. This approach is known as the conductive boundary model [3].

Often the detailed physics within the skin are of interest and need to be modeled, e.g. when investigating the impact of changes in the doping profile. This task is readily available in 1D by various (free) software tools. Multidimensional detailed modeling is however restricted to powerful commercial semiconductor simulation software, with drawbacks of significant user effort and much larger computational demand compared to lumped skin modeling.

A way to reduce the high effort for detailed cell modeling is to employ a three-step approach: 1) for each skin solve their characteristics in 1D, 2) determine their lumped properties, 3) apply these properties as boundary conditions for solving bulk carrier transport. Such a *multiscale* approach was shown to greatly improve speed of 1D cell simulations in [4]. For 2D/3D simulations one can combine different software tools, e.g. using EDNA2 [5,6] to determine the skin's

* Corresponding author.
E-mail address: andreas.fell@ise.fraunhofer.de (A. Fell).

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$J_{0,skin}$ and R_{sheet} as inputs for Quokka2 [2]. However, limitations of this approach are:

- Injection dependence of the recombination is complicated to account for, and thus usually neglected
- Vertical potential difference within the skin is neglected (e.g. from thin insulator layer or space-charge-region)
- Difficulty to consistently account for non-ideal collection of carriers within the skin, i.e. the skin's collection efficiency
- Prone to systematic mistakes due to using different tools (e.g. inconsistent $n_{i,eff}$ model, inconsistency of generation profile and skin depth)

This work alleviates those limitations by a) introducing a generally valid parameterization of the skin characteristics, and b) implementing both a 1D detailed "skin solver" and the multidimensional bulk solver in a single software tool, namely Quokka3. Notably, Quokka3 can handle multiple (full-area or local) skin features. They can individually be defined either by lumped inputs or by detailed inputs for the multiscale approach, allowing the user the option to choose just the right level of detail for a specific modeling task.

2. General skin parameterization

From a multidimensional numerical modeling perspective, a lumped skin is treated as a single-element-deep surface mesh, see Fig. 1. When using quasi-Fermi potentials as solution variables, as is the case in Quokka, the quasi-neutral steady-state solver requires a unique relationship between all face potentials and the face currents. That is, the element can be viewed as a black-box electrical circuit, which holds regardless of the details of the physics happening within the skin. The only assumption is that for significant lateral transport relative to the bulk, the majority carrier potential φ_{skin} is assumed to be constant within the main conductive region of the skin. This is the case e.g. within a highly doped near-surface region, or within the transparent conductive oxide (TCO) layer in a hetero-junction cell design. The assumption generally holds well for most typical crystalline silicon solar cell skins, in particular because of typical skins being *thin*, as can be perceived by the following:

- The assumption of a uniform φ_{skin} is only important for lateral current transport: for an effectively non-conductive skin, φ_{skin} denotes the potential only at the actual surface.
- To achieve significant lateral conductance, the vertical conductance of a thin region becomes very high, prohibiting significant vertical potential gradients.
- Most commonly only one type of carrier can have a significant lateral conductance within the skin, meaning that the skin can be assumed either purely *n*-type, *p*-type or non-conductive (neglecting some special cases, e.g. a "buried emitter").

For parameterizing the black-box characteristics, an equivalent

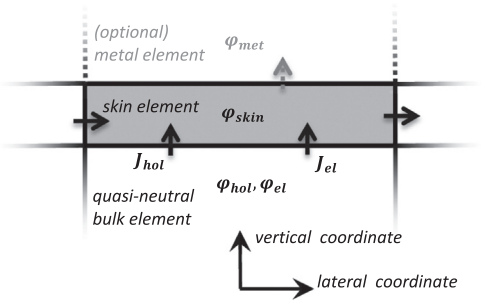

Fig. 1. Sketch of a single skin element within a 2D discretization for a numerical solver.

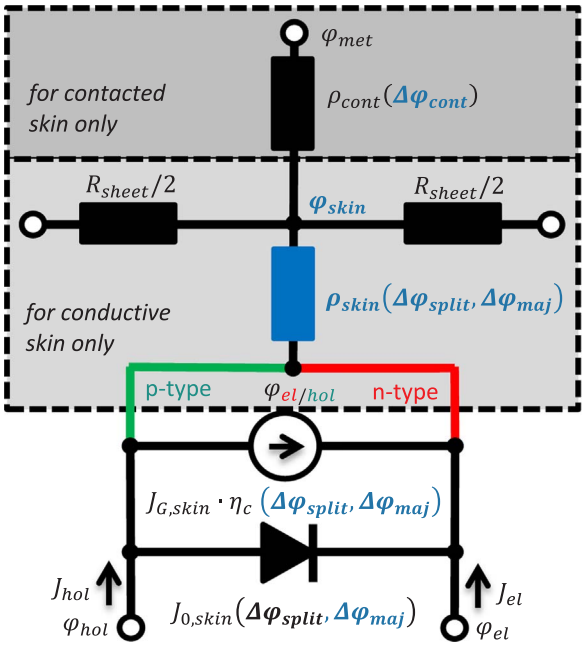

Fig. 2. Equivalent circuit model for a skin element; blue colour indicates the extensions to the conductive boundary model, accounting for vertical resistance and potential dependence of all parameters.

circuit model is applied, see Fig. 2. It extends the conductive boundary model by a) adding a vertical resistance ρ_{skin} between the bulk and the skin, and b) adding full potential-dependence (i.e. injection dependence) to all parameters. With the further assumption of being able to superimpose vertical and lateral current transport, which holds well for the same reasons given above, the main parameters are generally dependent on two potential differences only: i) the bulk-side quasi-Fermi potential split $\Delta\varphi_{split} = \varphi_{el} - \varphi_{hol}$, and ii) the vertical majority carrier potential difference $\Delta\varphi_{maj} = \varphi_{skin} - \varphi_{maj}$. For contacted skins, the additional metal contact resistivity ρ_{cont} depends (only) on the metal contact potential difference $\Delta\varphi_{cont} = \varphi_{met} - \varphi_{skin}$.

Generation of carriers within the skin is accounted for by the generation current density $J_{G,skin}$. Although not necessary from the black-box perspective, the lumped parameters become more meaningful if the skins's collection efficiency η_c is applied to $J_{G,skin}$. This way the recombination of carriers being generated within the skin is separated from the recombination of bulk-side carriers defined via $J_{0,skin}$, which enables a better definition of a texture multiplier as discussed in Section 3.3.

Note that while these lumped parameters are not always physically meaningful, they are generally valid as parameters also for arbitrarily complex skins. For example, ρ_{skin} can become negative to account for the voltage from a thin top-cell in a tandem configuration.

3. Implementation in Quokka3

3.1. Improved multidimensional quasi-neutral bulk (qn-bulk) solver

For solving multidimensional carrier transport in the bulk, the same efficient model as in Quokka2 is implemented, which most notably uses the quasi-neutrality assumption for omitting the need to solve the Poisson equation [2]. This model has been successfully validated to be accurate for typical silicon solar cells by comparisons against full detailed semiconductor device simulations [7,8]. In addition to Quokka2, which applies the common conductive boundary approach, Quokka3 enhances the qn-bulk solver by: i) a large performance boost via a rebuild in C++ and using PETSC [9] as a state-of-the-art library to solve the resulting system of nonlinear equations, ii) including an additional conductive layer on top of the skin layer at the front and rear