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Theoretical investigation of carrier-selective contacts featuring tunnel oxides by means of numerical device simulation

Heiko Steinkemper*, Frank Feldmann, Martin Bivour, Martin Hermle

Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstrasse 2, 79110 Freiburg, Germany

Abstract

Recently, a variety of different n-type Si solar cells with carrier-selective contacts featuring tunnel oxides achieving remarkable cell results has been presented. Theoretical investigations on this topic are rare, especially simulations actually accounting for tunneling through the oxide interlayer. In this work we investigate the influence of different parameters affecting the passivation quality and thus the device performance by means of numerical device simulation. Thereby, a fundamental understanding of solar cells with carrier-selective contacts featuring tunnel oxides is generated which is essential to further develop this promising technology.

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Keywords: Device simulation; numerical simulation; tunneling; tunnel oxide, carrier-selective contacts

1. Introduction

In the last year, different n-type Si solar cells with carrier-selective contacts featuring tunnel oxides have been presented [1-3]. All concepts feature high open circuit voltages of up to 739 mV [2] due to the good passivation properties of the oxide layers and high conversion efficiencies of up to 24.4 % [4] have been reached. Experimentally different approaches for the passivated contact are presented. Especially the doped Si layer can be amorphous [2], polycrystalline [3] or partially crystalline [4]. Beside the remarkable technological results there have not been a lot of theoretical investigations on this topic. A recent theoretical investigation of solar cells featuring

* Corresponding author. Tel.: +49-761-4588-5097; fax: +49-761-4588-9250.
E-mail address: heiko.steinkemper@ise.fraunhofer.de

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oxide interlayers has been carried out under the assumption that the current transport is dominated by carrier transport through oxide pinholes rather than by tunneling through the oxide layer [5]. In this work, since tunneling is expected to be efficient for very thin oxides (< 20 Å) [6] and some of the cell concepts feature ultra-thin oxide layers (12-15 Å [2] and 14 Å [1]), we assume that current transport is a result of carrier tunneling through the ultra-thin oxide layer.

The investigation of the contact quality of tunnel oxide passivated electron contacts is carried out performing numerical device simulations using Sentaurus Device [7]. In this work we will focus on the simulation principles (including details on the optical simulation) and the basic results concerning the recombination properties by means of an analysis of the open circuit voltage.

2. Simulation setup

The here investigated device is based on the electron selective TOPCon approach of Ref. [4]. The optical simulation as well as the electrical simulation are performed with Sentaurus Device [7]. Using such a complex device simulation environment is essential for the detailed investigation of the rear side properties of the solar cell as presented in this work, featuring thin layer stacks, complex band structures and carrier tunneling.

2.1. Optical simulation

The optical simulation is performed using a 3D symmetry element representing a quarter (upright) pyramid of the front surface texture of the modeled solar cell. Front metal contacts are not actually modeled in the optical simulation. The optical shading is considered in the electrical simulation by scaling the optical generation in the device.

Sentaurus Device uses a combination of transfer matrix model for thin layers like the anti-reflection coatings (ARC) at the front and raytracing. The cell features a double ARC at the front on top of a thin Al_2O_3 passivation layer. The corresponding layer thicknesses are listed in Table 1. The complex refractive indices of the MgF_2 at the front and the Si layer at the rear are based on experimental data measured at the Fraunhofer ISE, the materials of the remaining thin layers are taken from the material database of Sentaurus Device.

Table 1. Materials and corresponding thicknesses of the thin layer stacks (front and rear) used in the optical simulation.

Layer	Material	Thickness
Front ARC 1	MgF_2	100 nm
Front ARC 2	SiN	50 nm
Front passivation	Al_2O_3	10 nm
Rear tunnel oxide	SiO_x	1.5 nm
Rear Si layer	a-Si(n)	20 nm

The rear of the device featuring a tunnel oxide was simulated using the tilted mirror approach [8, 9] which accounts for additional surface roughness of silicon solar cells coated with dielectrics when using the transfer matrix formalism.

The optical and the electrical simulation are coupled using a 1D photo generation profile. This 1D profile is created from the 3D optical simulation by integrating over layers of equal distance perpendicular to the surface of the front texture. This is done for each wavelength and then the depth dependent total optical generation (shown in Fig. 1) is calculated depending on the irradiation spectrum, in this case the standard AM1.5G solar spectrum. The front texture is not actually modeled in the electrical simulation and the 1D generation profile is applied to an approximated, planar device.