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Investigation of selective junctions using a newly developed tunnel current model for solar cell applications

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ABSTRACT

Carrier transport through a tunnel barrier was modeled and implemented in the numerical device simulator AFORS-HET, which allows calculating the tunnel current between two semiconductor layers or between a metallic contact and a semiconductor layer. Rectangular barriers have been considered, for which an exact quantum solution for the transmission probability can be derived. The implementation in the simulation program was made by approximating the tunnel-interlayer as a "membrane" which modifies the current at the semiconductor/tunnel layer interface, without the need of inserting an additional insulator layer. It is demonstrated that this approximate description of the structure allows to simulate solar cells where tunneling across an insulator plays an important role. The model is then used to investigate new hole collector designs based on a tunnel oxide. It is shown, that the tunnel layer increases the selectivity of the contact for hole extraction, such that very high power conversion efficiencies can be reached.

1. Introduction

Intuitive, open-source simulation programs like AFORS-HET [1] or PC1D [2] allow easy access to one dimensional simulations of solar cells and other (opto-) electronic devices. They are extremely convenient in most cases because they are easy to handle and still provide a sufficiently precise description of most physical phenomena that are relevant for the device. Detailed studies of the influence of technologically relevant parameters of solar cells such as amorphous silicon/crystalline silicon (*a*-Si:H/*c*-Si) heterojunction cells have been carried out using such simulators, and have been very helpful for understanding and improving such devices. Among others, interface defect densities [3], transparent conductive oxide (TCO) work function [4], and interfacial band offset [5] have been studied in this way.

Silicon wafer based solar cells have been improving over the years, and reach now remarkable efficiencies with a record at 25.6% power conversion efficiency [6]. Such high performance can be obtained only if photo-generated electron–hole pairs can be extracted with negligible losses, thus requiring excellent selectivity and metal–semiconductor contact schemes. Furthermore from an industrial point of view, a cell structure gains in attractiveness if it can withstand high temperature steps mandatory in standard silicon technology for homojunction formation and contacts. Starting from these two assessments, research activities on silicon wafer based solar cells tend to merge standard industrially robust homojunction technologies with high efficiency *a*-Si:H/*c*-Si heterojunction cells. Recently, new junction architectures have appeared where an ultra-thin silicon oxide based passivation layer is used for *c*-Si surface passivation and to improve the electron/hole selectivity, and thus solar cells performance. For example, we investigated the concept of an *a*-Si:H/*c*-Si heterocontact, where the (i)*a*-Si:H passivation layer is replaced by an ultra-thin oxide layer [7]. The company Silevo also proposes a structure close to that one [8,9]. In a similar way, Feldman et al. have reported on the Fraunhofer ISE TopCon concept [10,11], which consists of a poly-*c*-Si/*c*-Si solar cell structure with a silicon oxide interfacial passivation layer. All these structures allow having an abrupt carrier collector/absorber interface, thus yielding potentially higher carrier selectivity. In addition, the insertion of a silicon oxide buffer layer reduces the interface density of states such that higher open circuit voltage values (V_{oc}) are expected. Regarding light trapping, the front carrier collector might be more transparent than in *a*-Si:H/*c*-Si structures, resulting in higher short-circuit current values (J_{sc}). However, since an insulator barrier that has to be overcome by tunneling is present in these devices, current transport might

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be the key issue for maximizing their performance: it is still unclear how high fill factor (FF) values can be reached with such concepts.

Up to now, very few theoretical studies have shed light on the behavior of such cells, and most of the studies report results on Metal–Insulator–Semiconductor structures (MIS) [12]. The lack of simulation studies is probably partly due to the fact that such works require the use of expensive and complex simulation tools; indeed we are not aware of any free programs allowing for the accounting of tunneling through an insulator layer. To partly solve this issue, it is necessary to provide numerical tools able to simulate these new structures. This is what justified the implementation of tunnel current models in AFORS-HET, and the new release of this program for free-on-demand access to the photovoltaic community (see Appendix B).

In Section 2 we give details on which models we consider for the tunnel current, as well as explanations on how they are implemented in AFORS-HET. In Section 3 we comment on the validity and limits of this tool. Finally in Section 4 we simulate a solar cell whose emitter structure is similar to the one described in [10], and discuss the suitability of such structures for photovoltaic devices.

2. Tunnel model: the "membrane" concept

2.1. General considerations

Accounting for tunneling in a self-consistent manner is not straightforward in semi-classical simulation programs, due to the non-locality of this quantum phenomenon. Yang et al. developed a model to account for tunneling through a spike in either the valence or conduction band resulting of band discontinuities at a heterojunction between two semiconductors [13]. Tunneling is taken into account in a semi-classical formalism, where Maxwell–Boltzmann statistics is considered instead of the Fermi–Dirac statistics; this results in an interface current J_{int} which is the product between the thermionic emission current and $(1+\delta_{Yang})$:

$$J_{int} = A^*T^2\left(1+\delta_{Yang}\right)\left(\frac{n_1}{N_{c,1}} - \frac{n_2}{N_{c,2}}e^{-\frac{\Delta E_c}{k_B T}}\right), \quad (1)$$

where A^* is the minimum of Richardson constants of both semiconductors, T is the temperature, n_i and $N_{c,i}$ are respectively the electron concentration and conduction band effective density of states in material i, ΔE_c is the conduction band offset at the interface and k_B is the Boltzmann constant. The term δ_{Yang} includes tunneling probabilities at all energies along the considered band close to the interface:

$$\delta_{Yang} = \frac{\exp\left(\frac{E_c(0^+)}{k_B T}\right)}{k_B T}\int_{E_{min}}^{E_c(0^+)} T(E)\exp\left(-\frac{E_x}{k_B T}\right)dE, \quad (2)$$

where $E_c(0^+)$ is the conduction band edge energy on the right of the interface, E_{min} is the minimum energy allowing for tunneling in the conduction band and $T(E)$ is the transparency of the barrier electrons have to come across. More detailed equations can be found in [13]. A typical situation where Yang's model applies is presented in the inset in Fig. 1.

In Yang's model, the tunneling current is added to the interfacial thermionic current, making the implementation of tunneling local. A more accurate model has been developed by Verschraegen et al. [14], where tunneling is accounted in a non-local way: tunnel current components are added continuously in the structure, and not only at the interface. However, Verschraegen's work showed that Yang's model is a rather good approximation.

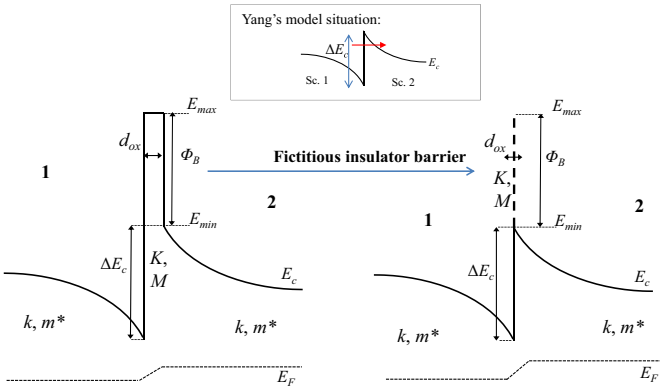

Fig. 1. Band diagram (focused on the conduction band) for a semiconductor/insulator/semiconductor structure. k_i and K are the wave vectors in semiconductor i and in the insulator respectively; m^* and M are the tunneling effective masses in the semiconductors and in the insulator respectively. d_{ox} is the insulator thickness. Left: structure considered for current calculations. Right: structure as implemented in AFORS-HET is no real insulator layer is inserted, but the interfacial current accounts for a fictitious insulator barrier. Inset: tunneling through a spike in the conduction band at a hetero-interface described by Yang's model.

In a similar way, we developed a local model to account for tunneling through an insulator layer. The insulator layer is included in the structure not as an additional layer; instead, the electrical current through the interface between the two semiconductors is actually the current that would flow through a fictitious insulator layer by tunneling. Instead of simulating explicitly the layer, i.e. solving the semiconductor equations in it, the insulator layer is treated analytically, taking the input parameters for the analytic calculation from the semiconductor/semiconductor interface grid points (see Fig. 1).

In the following, the equations describing the tunneling current are developed.

2.2. Tunnel barrier at the semiconductor/semiconductor interface

In this section we present the equations implemented in the simulator AFORS-HET to model tunneling through an insulator layer sandwiched between two semiconductors. Such a situation is depicted in Fig. 1. We make the following assumptions: (i) the tunneling process is elastic, i.e. the charge carrier which undergoes tunneling does not loose energy in the process, (ii) the tunneling effective mass is the same on both sides of the barrier, and (iii) the energy barrier is considered rectangular. The derivation can be found in most of the quantum mechanics textbooks (see for example [15]) and is reproduced in the Ph.D. thesis of Ref. [16,17].

The starting point for the electron tunnel current $J_{e,tun}$ calculation is the so-called Tsu–Esaki formula [18]

$$J_{e,tun} = \frac{4\pi q m^*}{h^3}\int_{E_{min}}^{+\infty} T(E)N(E)dE, \quad (3)$$

where E_{min} is the minimum conduction band edge energy allowing for tunneling (see Fig. 1), and is defined through the band alignment. q is the elementary charge, m^* is the tunneling effective mass in the semiconductors and h is Planck's constant. The transparency $T(E)$ of the barrier gives the probability for an electron with the energy E to tunnel through the barrier. In the case of a simple rectangular shaped barrier, an analytical expression for $T(E)$ can be derived from the plane wave approximation. We give here only the final equations [15–17]: