First investigation of quantum effects in heterojunction solar cells

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***Abstract*– This paper focuses on the impact of quantum effects in a-Si:H / c-Si heterojunction solar cells simulation. A simulation flow is presented, in which a self-consistent Poisson-Schrödinger approach is coupled with classical physics simulations. It is shown that quantum effects have a significant impact on the calculated charge description at front a-Si:H / c-Si interface and appear mandatory for accurate a-Si:H parameters extraction and confident heterojunction solar cell simulation results.**

I. INTRODUCTION

Amorphous (a-Si:H) / crystalline (c-Si) Silicon-based heterojunction (HET) appears as the most promising technology for reaching high solar cell efficiency with reduced fabrication costs [1]. From mid-90's to early 2000's, Heterojunction with intrinsic Thin-layer (HIT™) solar cells efficiency increased from 14 up to 21% [2], mostly thanks to process development and optimization.

Since 2000, further increase requires a better understanding of the physical phenomena occurring in ultra-thin a-Si:H layers and at a-Si:H / c-Si interfaces, together with a better knowledge of a-Si:H material properties. In particular, the identification of transport mechanisms in a-Si:H appears as the most critical issue in the literature. So far several models have been proposed for conduction through these layers [3] but the true mechanism remains unclear and seems to be process dependent [4-6].

HET solar cells consist of a n-doped c-Si substrate sandwiched between doped and buffer a-Si:H layers, leading to the creation of an inverted hole-rich layer at c-Si front interface. Prior to any a-Si:H transport modelling, attention has to be paid to the incoming charge description in the inverted channel at a-Si:H / c-Si interface, which has been surprisingly poorly investigated yet.

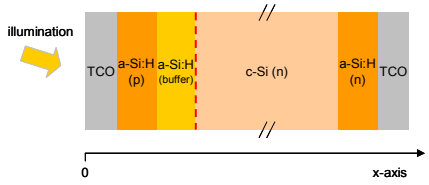

FIGURE 1. HET solar cell considered in this work, featuring ultra-thin a-Si:H layers (n, p and buffer, a few nm thick), TCO contact layers and c-Si (n-type) base.

In this paper, we propose to measure the influence of quantum effects at c-Si interface on the overall macroscopic behaviour of the solar cell, and to give a ruling on the relevance of such microscopic modelling in HET solar cell simulation.

II. MODELLING

In this work, we consider a state-of-the-art HET structure fabricated at INES (National Institute for Solar Energy) [7]. Because of the electric field created by the heterojunction, an inverted hole channel is present at c-Si interface (dashed red line, Fig. 1), in which hole carriers are confined in a 2D-gas prior to their motion through a-Si:H layers.

Solar cell modelling requires 2D simulation tools (e.g. Silvaco Atlas) in order to account for 2D effects (contacts shadowing, lateral conduction…). In such software, the charge is obtained by solving self-consistently both Poisson equation and Boltzmann transport equations (drift-diffusion model) [8]. Accounting for the quantum nature of carriers would require solving self-consistently these equations together with Schrödinger equation, which is impossible with Silvaco Atlas or too much time consuming with any other simulation program.

In order to bypass this issue, a pragmatic approach has been considered:

1/ Structure potential and quasi-Fermi levels position have been calculated using Silvaco Atlas (i.e. classical physics).

2/ Then, Schrödinger equation has been applied on the classically computed structure in order to calculate hole and electron concentrations [9].

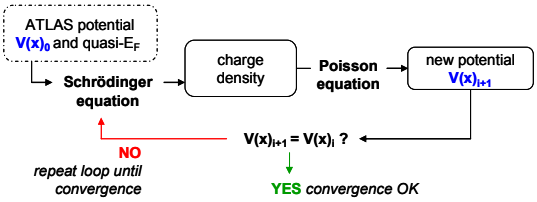

FIGURE 2. Convergence scheme of the self-consistent Poisson-Schrödinger simulation tool.

3/ As quantum charge concentration may differ from the classical charge computed by Atlas, modifications in the simulated potential profile are expected (Poisson equation). For that purpose, we developed a self-consistent Poisson-Schrödinger (PS) simulation tool, represented in Fig. 2 [10]. As Boltzmann transport equations are not included in PS simulations, we assume that the quasi-Fermi levels computed with Atlas are constant throughout PS resolution (i.e. not affected by quantum effects).

III. Results and Discussion

Silvaco Atlas simulations have been performed at different biases, under dark and illumination conditions. For the sake of clarity, this work only refers to a zero-biased cell under illumination (i.e. short-circuit current condition).

Fig. 3 compares the band structures and charge densities computed with Silvaco Atlas and after Poisson-Schrödinger self-consistent resolution. When the quantum nature of carriers is accounted for, we observe that the maximum density of charge is shifted 1nm away from a-Si:H (see the solid blue line) leading to a deserted area (also known as *darkspace*) near the interface. Moreover, it appears that the total charge calculated by PS simulation (i.e. charge density integrated along x-direction) is 1.5 times lower than in classical Atlas simulation: it explains the small modification of the potential profile shown in the gray circle, which is needed to fulfil both Poisson and Schrödinger requirements.

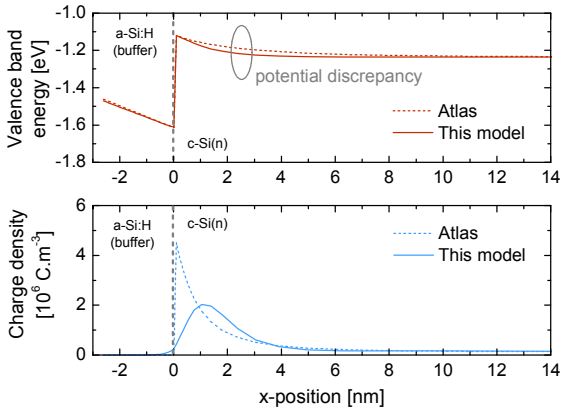

FIGURE 3. Band structure and charge density at a-Si:H(buffer) / c-Si(n) interface, considering classical physics (Silvaco Atlas, dashed lines) or quantum mechanics (this model, solid lines).

As can be seen on Fig. 4, charge distribution over energy is also strongly impacted by quantum confinement: the hole gas is no longer 3D (as simulated by Atlas), and quantized states at the interface lead to a discontinuous 2D density-of-states, much lower than the classical 3D DOS. On one hand, it explains the previously observed charge differences between Atlas and quantum simulations, and, on the other hand, it is expected to have a strong impact on transport modelling through amorphous layers.

IV. Conclusions

While quantum effects do not strongly modify HET cell band bending, and thus the simulated V_{oc} value, they have a significant impact on transport modelling through a-Si:H. As charge distribution along both energy and spatial coordinates are impacted, attention has to be paid to proper account for quantum effects prior to any a-Si:H parameters extraction.

When characterizing a-Si:H, parameters are extracted by fitting electrical characteristics with appropriate transport models (direct tunnelling, trap-assisted-tunneling…), which are directly linked to the incoming charge description [11, 12]. While classical physics would always allow to reproduce experimental HET characteristics with *effective* parameters, accounting for quantum effects appears mandatory for an accurate extraction of a-Si:H parameters, which would lead to confident predictive simulations for HET solar cells optimization.

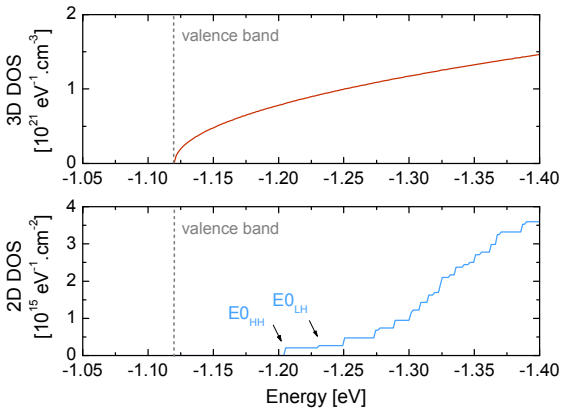

FIGURE 4. Valence band densities-of-states considered in classical (3D-gas, red line) and quantum simulations (2D-gas, blue line). $E0_{HH}$ and $E0_{LH}$ denote the first heavy (HH) and light holes (LH) quantized states.

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