Quasi 1D multi-physics modeling of silicon heterojunction solar cells

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***Abstract*—Silicon based technology continues to mature and move steadily towards the auger limited maximum efficiency (~29%). In particular silicon heterojunction technology currently holds the world record for silicon based single junction cells. Optimization of heterojunction solar cells now requires a concentrated and deep understanding of the physics of transport. In this paper we present a multi-physics/multiscale approach to understanding and analyzing transport in silicon heterojunction solar cells. We self-consistently couple a traditional drift-diffusion model to an ensemble Monte Carlo and kinetic Monte Carlo to create a multiscale solver that is capable of including high field effects present at the a-Si/c-Si heterointerface and the nuances of defect assisted transport through the a-Si:H(i) buffer layer.**

Keywords— silicon, amorphous silicon, heterojunction, solar cells, modeling, simulation, multiscale

I. INTRODUCTION (*HEADING 1*)

Silicon solar cells have several characteristics which are crucial for photovoltaic technologies, such as: Si is abundant, easily scalable, non-toxic, and can be fabricated at low temperatures at relatively low cost. Improving efficiencies of Si based technologies is a key step to cement the use of photovoltaics as a ubiquitous source of energy. In particular, silicon heterojunction (SHJ) solar cells comprised of crystalline silicon (c-Si) substrates and thin amorphous silicon (a-Si) passivating layers have demonstrated continuous increase in conversion efficiencies [1]. Most recently, Kaneka Corporation demonstrated a world record efficiency of ~26.6% for a SHJ based on a-Si and c-Si [2].

The drift-diffusion(DD) model has most often been used to simulate and analyze electrical characteristics of solar cells. However, the DD model is a semi-classical model that is accurate only when systems are in near-equilibrium and under the influence of low electric fields. As we move towards 2nd and 3rd generation solar cells [3], novel device designs and new materials often lead to scenarios where the physics is no longer truly semi-classical. In this paper, we present a multi-physics/multiscale methodology that is used to study transport in an a-Si/c-Si heterojunction solar cell shown in figure 1, also referred to as a HIT (heterojunction with intrinsic thin layer) cells [4]. Our work primarily focuses on studying interfacial transport across the a-Si/c-Si heterointerface in a SHJ solar cell as the quality of this interface modulates device properties such as fill factor (FF), open circuit voltage (V_{oc}), short circuit current (J_{sc}) and efficiency. There are two regions in the HIT cell which particularly require careful consideration: 1) The high field region at the intrinsic a-Si (a-Si:H(i)) and c-Si heterointerface, and 2) the a-Si:H(i) buffer layer which provides passivation. The built-in potential at the a-Si/c-Si heterointerface creates sharp band bending together with an abrupt band discontinuity, which results in high fields. This leads to a non-Maxwellian non-equilibrium energy distribution of photogenerated carriers at the heterointerface [5], which violates some of the assumptions made to derive the DD model from the Boltzmann transport equation (BTE). The high fields exist over a few 100 nm's and the scattering mechanisms that govern the physics of the energy distribution of carriers are of the order of 10^{-12} s. Previously, we have developed an ensemble Monte Carlo (EMC) to capture the effect of photogenerated carriers under high fields [6]. Photogenerated carriers at the a-Si:H(i)/c-Si interface need to traverse an amorphous layer before they can be collected. Transport across this layer is primarily governed by a 'hopping' mechanism where the carriers undergo many defect to defect transitions. Crandall *et al.* experimentally verified this mechanism by conducting transient capacitive measurements [7]. In our studies, we developed a kinetic Monte Carlo (kMC) simulation tool to simulate this 'hopping' mechanism [8]. Our simulations indicated that the time associated with each defect interaction can range from $10^{-12} \rightarrow 10^{-6}$ s. In this paper we describe our strategy to couple the various solvers.

II. THEORETICAL MODEL

In this section we will describe the different solvers that are utilized to isolate and study various regions of the device. Fig. 1 shows a schematic diagram of a silicon heterojunction (SHJ) solar cell; the different solvers operating in different areas of the cell are highlighted in different colors.

As mentioned in the introduction, the three solvers that we developed are drift-diffusion, ensemble Monte Carlo and kinetic Monte Carlo to study the physics of transport in various regions of the device

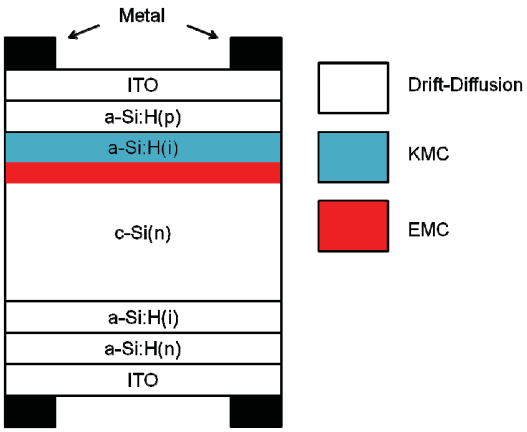

Fig. 1. Schematic diagram of a SHJ solar cell highlighting the different simulation domains.

A. *Drift-Diffusion (DD)*

We developed a one dimensional DD solver to model the electrical characteristics for heterostructure solar cells. The DD model entails solving the steady state semiconductor continuity equations in conjunction with Poisson's equation. The DD model is initially applied to the entire device structure to calculate electric fields, potentials and current. However, due to the assumptions that are inherently present in the DD model, these results are only accurate for low field scenarios. There is an inherent assumption that the carriers always exist at thermal equilibrium or in other words, the carriers have a Maxwellian energy distribution (~39 eV). However, due to the presence of the a-Si and c-Si heterointerface, there exists high fields at the heterointerface which violates the low field assumption. Thus, the purpose of the DD solver in the multiscale framework is to model low field effects. Low fields exist in the quasi-neutral areas of the solar cell such as the absorber which can be >100 μm thick. Steady state phenomena such as recombination is dominant in bulk c-Si where the recombination lifetime ~ 2-4 ms.

B. *Ensemble Monte Carlo(EMC)*

The EMC is applied to the a-Si/c-Si hetero-interface where high fields exist. The high field region spans ~100-200 nm and the transport is primarily limited by scattering which happen over a pico second scale. We assume that there is no recombination in this region. Considering that the EMC is applied to the front interface (as shown in Fig. 1) which is <20 nm away from the contact and the diffusion length is in order of 10^{-6} m (microns); this is a good assumption. Thus the function of the EMC is to capture the effect of high field on the charge distribution of holes near the interface.

As the structure shown in Fig. 1 has a p doped a-Si emitter layer (a-Si:H(p)) and an intrinsic a-Si buffer layer (a-Si:H(i)); the photogenerated carriers collected at the front contact are holes. Thus, we developed a 3 band EMC for holes which considers warping for the light hole and heavy hole bands whilst the spherical band is considered to be parabolic. We also include non-parabolicity for the light hole and heavy hole bands.

C. *Kinetic Monte Carlo (KMC)*

Another area of the device where a purely semi-classical description of transport might be found lacking is in the a-Si:H(i) buffer layer. The a-Si layer consists of defect states below the conduction band edge (localized defect states) and around midgap (midgap defect states) which can play a crucial role for transport of carriers. Thus, we implemented a KMC solver in the a-Si:H(i) buffer layer (~10 nm thick) to study defect assisted transport. As the transport is dependent on defect emission and defect capture times, defect assisted transport can range from $10^{-6} \rightarrow 10^{-12}$ sec based on carrier energy and defect density.

D. *Drift Diffusion-Monte Carlo (DD-MC)*

The previous sections (IIA-IIC) outline the applicability of the DD, EMC and KMC solvers. It is important to note that each solver finds its applicability over a vastly varying spatial range and the dominant transport mechanism occurs over vastly different time scales in each domain. In this paper, we seek to outline an approach to combine the DD and MC solvers. Coupled DD-MC solvers have previously been applied to analyze hot electron effects in MOSFET's [9]. However, as far as we know this technique has never been applied to a bi-polar problem which exists in a solar cell.

III. Results and Discussion

Fig. 2 shows the energy band diagram of a SHJ solar cell as calculated by the DD solver. Fig. 3 shows the front emitter of the energy band diagram where the high field area is encircled.

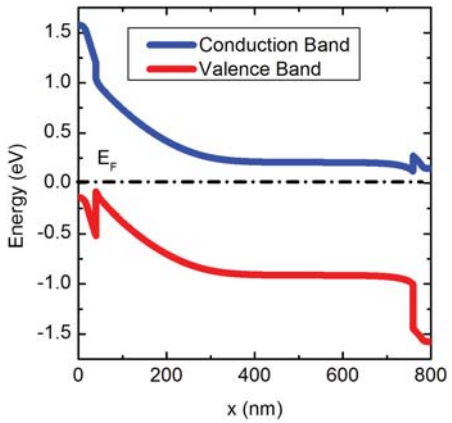

Fig. 2. Energy band diagram of a SHJ solar cell as calculated by the DD model.

In Fig. 3, B1 and B2 mark the boundaries of the EMC region. Boundary B2 is placed at the a-Si:H(i)/c-Si interface where the electric field is close to the peak electric field in the device and the DD assumption of low field is violated. Boundary B1 is placed in the quasi-neutral region of the device where the DD solution and EMC solution converge due to low electric fields. Once the DD solver calculates the initial values of electric fields, current and potentials; an EMC window is opened in the device where carriers are injected into the EMC domain based on the initial DD current. The boundary conditions at boundaries B1 and B2 are crucial as it

is very important as to inject the carries with the right energy and wave vector distribution [10]

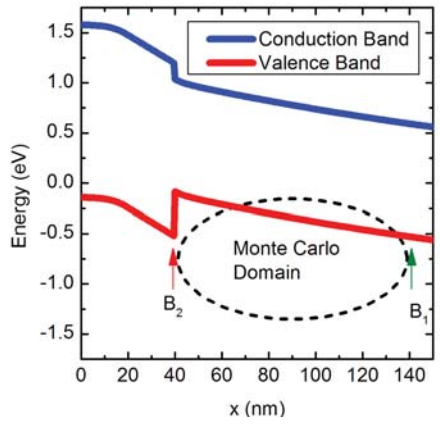

Fig. 3. Energy band diagram of the front emitter interface for a SHJ solar cell. B1 and B2 mark the boundaries of the Monte Carlo domain which encompasses the high field region.

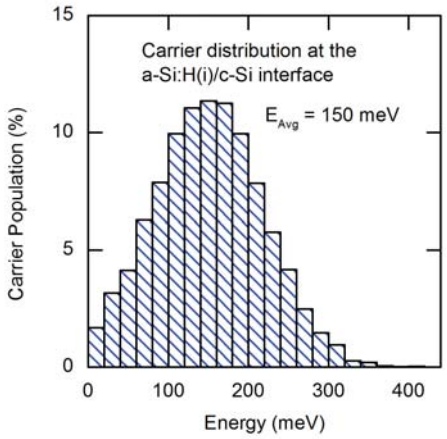

Fig. 4. Energy distribution of the carriers at the a-Si:H(i)/c-Si heterointerface.

The current calculated from the DD solver is injected into the EMC domain. The EMC domain calculates the energy of the photogenerated holes at the a-Si:H(i)/c-Si heterointerface. Fig. 4 shows the average energy of the hole distribution to be ~ 150 meV. This value is much larger that the value assumed by the low field assumption made by the DD model ~ 39 meV. As the photogenerated carriers encounter a potential barrier at the a-Si:H(i)/c-Si heterointerface, it is imperative to consider the energy of the carriers as it has a direct implication on the probability of tunneling across the barrier.

Fig. 5 shows the current that is extracted from the EMC domain. The slope of the cumulative charge vs. time plot gives the current (I); this divided by the cross sectional area give the current density (J). The carriers incident on the a-Si:H(i)/c-Si heterointerface are extracted based on thermionic emission and direct tunneling probability. We are currently working on a formulation which will include a "hopping" probability that is extracted from the KMC.

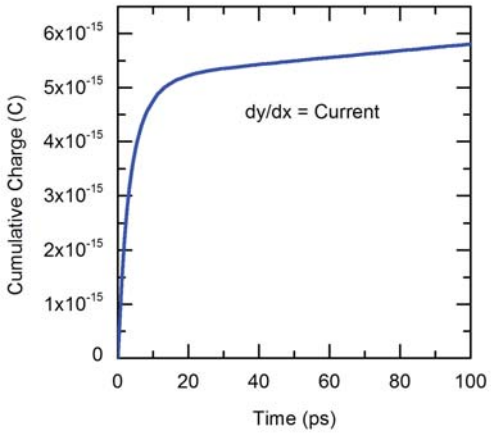

Fig. 5. Cumulative charge vs. time for charge extracted at the a-Si:H(i)/c-Si heterointerface from the EMC domain.

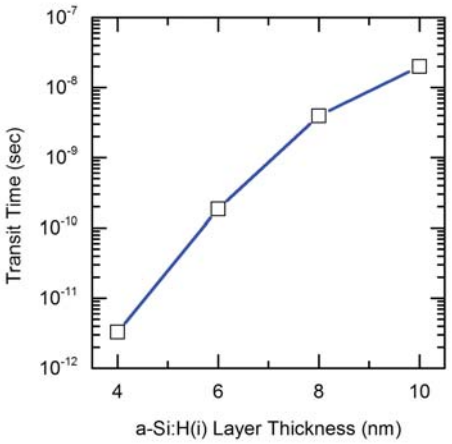

Fig. 6. Transit time vs. a-Si:H(i) layer thickness as calculated by the KMC solver.

Fig. 6 shows the transit time vs. a-Si:H(i) layer thickness as caluclated by the KMC solver. Our simulations indicated that the photogenerated carriers "hop" from defect to defect as they traverse the a-Si:H(i) buffer layer. Thus, the increase in thickness of the a-Si:H(i) buffer layer leads to an increase in transit time. This shows that the thickness of the buffer layer has a profound influence on photocurrent suppression at the heterointerface.

Fig.7 shows a comparison of the hole carrier density as calculated by the DD solver and the fully self consistently coupled DD-MC solver. Boundaries B1 (low field) and B2 (high field) mark the boundaries of the EMC domain. The hole carrier density calculated by the EMC (coupled with a global Poisson solver) is relatively smooth. This is a good indication of that the boundary conditions being applied are valid as there are no discontinuities which would indicate that physical laws are being violated. Our next step is to analyze

the quantitative difference between the I-V characteristics calculated by the DD solver and DD-MC solver.

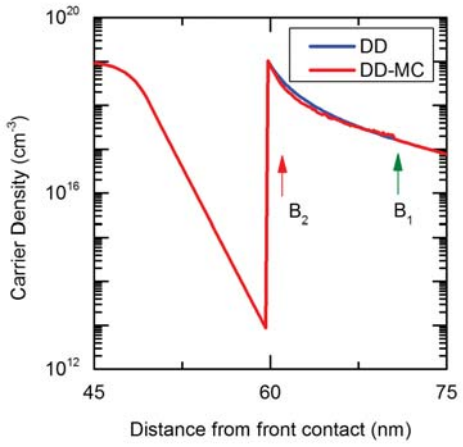

Fig. 7. Hole density as calculated by the DD and DD-MC solvers.

IV. Conclusions

Initial analysis of the SHJ device structure indicated that there are certain areas within the cell that cannot be accurately described by traditional semi-classical physics. Also, the nature of transport at in the quasi-neutral region, at the a-Si:H(i)/c-Si heterointerface and through the a-Si:H(i) buffer layer constitutes a multiscale problem due the vastly varying time and length scales. We applied a DD solver to model all the low field areas in the device where the properties are primarily dominated by the bulk lifetime, an EMC solver at the a-Si:H(i)/c-Si heterointerface to model the charge distribution under high fields and to take under consideration the quantum nature of transport at the heterointerface, and finally we developed a KMC solver to explicitly simulate defect assisted transport through the a-Si:H(i) buffer layer. Our primary findings were that, 1) there exists an energized carrier distribution at the a-Si:H(i)/c-Si heterointerface which has implications for transport across the potential barrier and 2) hopping is the primary mode of transport across the a-Si:H(i) buffer layer. In this paper we present a self-consistently coupled drift-diffusion ensemble Monte Carlo solver.

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