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A kinetic Monte Carlo study of defect assisted transport in silicon heterojunction solar cells

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The device performance of an amorphous silicon (a-Si)/crystalline silicon (c-Si) solar cell depends strongly on the interfacial transport properties of the device. The energy of the photogenerated carriers at the barrier strongly depends on the strength of the inversion at the heterointerface and their collection requires interaction with the defects present in the intrinsic amorphous silicon buffer layer. In this work we present a theoretical model to study the defect assisted transport of photogenerated carriers through the intrinsic amorphous silicon barrier. We implement the kinetic Monte Carlo (KMC) method which allows us to simulate the interaction of discrete carriers with discrete defects. This method allows us to study defect transport which takes place on a time scale which is too long for traditional ensemble Monte Carlo's to analyze. We analyze the injection and extraction of carriers via defects by calculating transition rates, i.e. probability of transition to defect states within the intrinsic amorphous silicon barrier. The KMC results allow us to quantitatively study the properties of the heterointerface barrier in terms of how it affects transport.

1 Introduction Photovoltaic cells based on a-Si/c-Si lead the charge towards the Shockley-Queisser efficiency limit for single junction solar cells. Last year a world record device efficiency of 25.6% was reported for Panasonic's trademark HIT cell. This cell featured a slight deviation from their traditional cell structure by incorporating interdigitated back contacts and improved methods of placing the a-Si layers on the crystalline silicon [1]. In the initial design of the heterojunction solar cell doped a-Si was placed on the c-Si absorber layer which lead to the creation of many interface states. This caused the short-circuit (J_{SC}), open-circuit voltage (V_{OC}), and efficiency to be much lower than expected. The addition of a hydrogenated intrinsic amorphous silicon layer between the doped amorphous emitter and the c-Si absorber layer provides the necessary passivation which prevents degradation of device performance due to interface states. Thus, the intrinsic buffer layer is paramount for realizing high V_{OC}'s, J_{SC}'s, fill factors and efficiencies [2].

Due to the novel structure of the device, the physics behind the transport behaviour is still a matter of debate. Commercial device simulators traditionally use methods such as drift diffusion to simulate device properties; which is a good model to simulate conventional device structures where the transport takes place in the semi-classical regime [3]. But the presence of a heterointerface and the barrier formed by the intrinsic amorphous silicon layer (see Fig. 1) together create an unconventional situation where assumptions made by the conventional drift diffusion model are no longer valid. Previous work by Ghosh *et al.* [4] has shown the effect of high fields on the carrier distribution at the heterointerface. In this work we explore and study the various mechanisms that govern transport of photogenerated carriers in the intrinsic amorphous silicon barrier. As the amorphous barrier is replete with defects the main mode of transport is via defects. We apply the kinetic Monte Carlo (KMC) method to study defect assisted transport by analyzing the interaction of discrete defects with discrete carriers. This method enables us to study not only the impact of various mechanisms such as thermionic emission, direct tunnelling, Poole-Frenkel (PF) emission, capture and emission from defects on the collection of photogenerated carriers, but the effect of various defect distributions on transport behaviour can also be evaluated.

2 Theoretical model Figure 1 shows a schematic diagram of an a-Si/c-Si HIT cell. The intrinsic amorphous barrier under consideration is considered to be 10 nm for all simulations. We conducted Silvaco ATLAS simulations for the given device at the maximum power voltage to calculate fields and potentials in the barrier region. Using the methodology outlined in [5], the energy distribution of the photogenerated carriers at the front a-Si/c-Si heterointerface was calculated using the fields provided by the Silvaco ATLAS simulations and an ensemble Monte Carlo (EMC) particle based method that simulates transport in the high field region at the heterointerface.

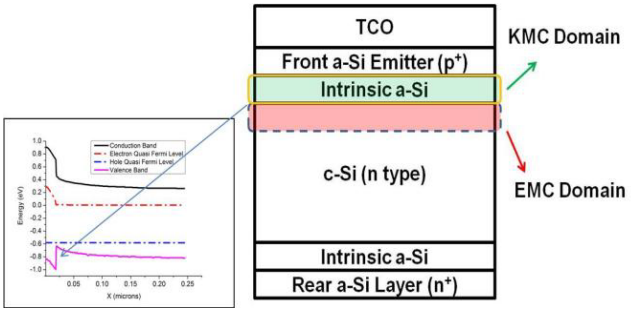

Figure 1 Schematic diagram of a HIT cell. The green region indicates the KMC domain (intrinsic a-Si) and the red region indicated the EMC region (c-Si absorber).

The carrier distribution calculated by the EMC is then used in the KMC domain where the carriers interact with the defects. At the beginning of the simulation run a defect distribution is generated in real space and energy space after which they are assigned occupation. We do not consider the effect of mid gap states in our simulations.

2.1 Kinetic Monte Carlo The KMC domain simulates the interaction of discrete defects present in the intrinsic a-Si barrier with the carrier distribution of the photogenerated carriers as calculated by the EMC. The carriers 'hop' through various localized defect states that are present in the barrier which are described by Eq. (1). These localized states or band tail states are created as a result of strained Si-Si bonds. There is certain probability that these strained bonds could break and create dangling bonds which create amphoteric mid gap states. A high enough density of dangling bond states can result in increased interface recombination limiting device performance. A 'defect pool' model exists to theoretically study and model dangling bond states [6] but is not considered in this work. Using Eq. (1), a discrete defect distribution is created which is uniformly distributed in real space and decays exponentially in energy from the band edge.

$$N(E) = N_{VBT} \exp\left(\frac{-\left(E - E^*\right)}{E_0}\right), \tag{1}$$

where E is the energy of the carrier, E^* is the band edge energy, E_0 is the characteristic decay energy of a-Si and N_{VBT} is the peak concentration of the density of states [7].

2.2 Transport mechanisms Once the EMC simulator calculates the energy distribution function (EDF) of the carriers at the interface, the carriers are ready to make transitions to defects within the barrier. This can be accomplished by calculating transition rates. The carriers are injected via a defect capture mechanism whereas they can be extracted via defect emission, Poole Frenkel emission or thermionic emission [8].

The carriers at the interface can be captured by defects elastically and inelastically via phonons as shown by Eq. (2):

$$\begin{aligned} R = &\sum_{p<0} c_0 N_E(E_p)\,\mathrm{f}(E_p) T(E_p, x) L_p(z) e^{\frac{\hbar\omega}{kT}} \\ &+ \sum_{p>0} c_0 N_E(E_p)\,\mathrm{f}(E_p) T(E_p, x) L_p(z)\,. \end{aligned} \tag{2}$$

In Eq. (2), $L_p(z)$ is the multi-phonon transitional probability, E_p is the energy of the coupled carrier phonon system, $T(E_p)$ is the tunneling probability to an energy E at a position x, $\hbar\omega$ is the optical phonon energy, and $N_E(E_p)$ is the density of states in the c-Si. The carriers can be extracted via defect emission as shown by Eq. (3) or by Poole-Frenkel (PF) emission as shown by Eq. (4), respectively.

$$\begin{aligned} R = &\sum_{p<0} c_0 N_E(E_p)[1 - \mathrm{f}(E_p)] T(E_p, x) L_p(z) \\ &+ \sum_{p>0} c_0 N_E(E_p)[1 - \mathrm{f}(E_p)] T(E_p, x) L_p(z) e^{-\frac{\hbar\omega}{kT}}, \end{aligned} \tag{3}$$

$$R = v \exp\left(-\frac{1}{kT}\left(E_D - \sqrt{\frac{e^3 F}{\pi\varepsilon_0\varepsilon_{opt}}}\right)\right). \tag{4}$$

In Eqs. (3) and (4), p is the number of phonons involved in the process and all other variables retain the same meaning as in Eq. (2). E_D is the defect depth, v is the lattice vibration frequency and F is the electric field. All other terms are physical constants that retain their traditional meaning. In the above treatment of PF emission, the carriers are emitted into the extended states parallel to the electric field.

2.3 Alternate defect distributions By varying the characteristic decay energy E_0 in Eq. (1) it is possible to generate different defect distributions in the intrinsic a-Si barrier. The characteristic decay energy is traditionally found to be 45 meV in literature (see Ref. [4]). But by varying the decay energy from 5 meV-100 meV it is possible to generate defect densities of 10^{18} cm^{-3} to 10^{20} cm^{-3}. These defect densities can mimic scenarios of μc-Si:H (micro-

crystalline silicon, low defect densities) and unhydrogenated amorphous silicon (high defect densities).

3 Results and discussion Figure 2 shows the non-Maxwellian distribution (E_{avg}=150 meV) that exists at the a-Si/c-Si heterointerface which is calculated by the EMC solver. This is the result of photogenerated carriers drifting through high fields which exist as a result of the heterointerface.

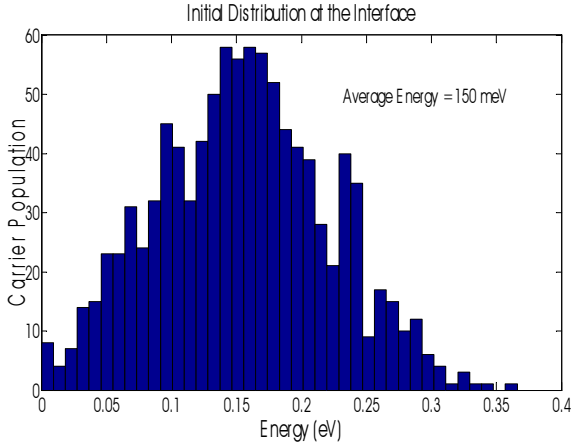

Figure 2 Energy distribution of carriers at the a-Si/c-Si interface.

The distributions of carriers after traversing the intrinsic a-Si:H is shown in Fig. 3.

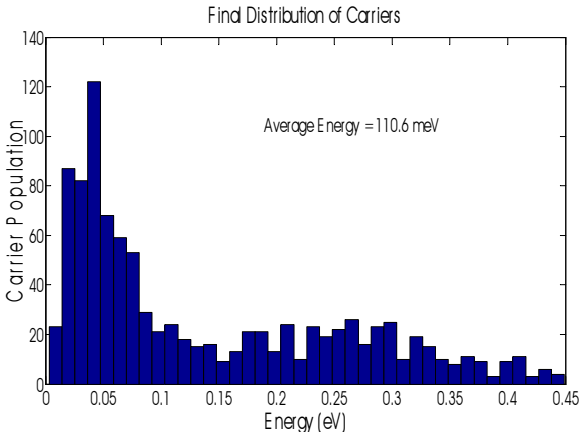

Figure 3 Energy distribution of carriers once they have traversed the intrinsic a-Si region and have been 'collected'.

Analysing the results in Fig. 3, we see that the average energy of the carrier distribution relaxes from 150 meV to 110 meV. This is a clear indication that the interaction of the carriers with the defects present in the barrier involves many phonon transitions. The carriers 'hop' through various defects via phonon transitions and consequently loose energy through emission processes.

Our simulations allow us to study the extraction mechanisms that result in the 'collection' of the carrier. Our simulations indicate that the dominant mechanism for extraction is a defect emission process. PF emission contribute to <2% of carrier extraction whereas thermionic emission contributes to <1% of carrier extraction. Another parameter our simulations can access is the average transit time τ_{avg} which is an indicator of the amount of current that is being suppressed within the device. Figure 4 shows the variation of average transit time vs. the average energy of carrier distribution.

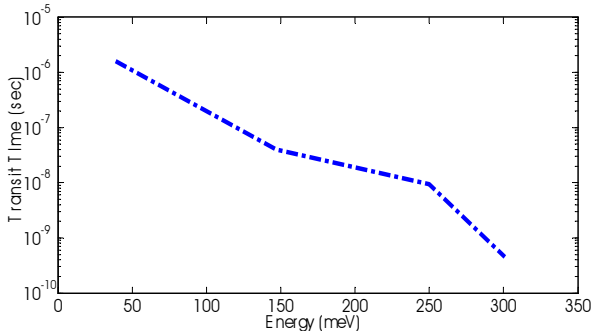

Figure 4 Average transit time vs. average energy of carrier distribution at the a-Si/c-Si interface.

4 Conclusions The KMC provides an excellent platform to study defect assisted transport in amorphous materials. In this work we have analyzed the role of various extraction mechanisms that lead to carrier collection. Also, this method can be utilized to study other dielectric/amorphous material systems which can be potentially incorporated into an a-Si/c-Si heterojunction device.

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