A Multi-Physics Model to Study Defect Assisted Transport in Amorphous Barrier Layers

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It is already well established that good surface passivation at the heterointerface in silicon heterojunction solar cells (SHJSC's) leads to high open circuit voltages (V_{oc}'s) and fill factors (FF's), and ultimately to high conversion efficiencies [1][2]. Hence, high device performance is obtained by using carrier selective contact (CSC) structures to optimize collection of photogenerated carriers [3]. In SHJSC's, CSC's usually consist of a transparent conducting oxide (TCO) and a doped (n or p type) hydrogenated amorphous silicon layer [a-Si:H(n/p)] on top of a crystalline silicon (c-Si) absorber (see Fig. 1). Traditionally, passivation layers based on intrinsic hydrogenated amorphous silicon [a-Si:H(i)] have been used between the doped a-Si:H and the c-Si in the highest efficiency cells, to create a low recombination contact.

In this work we use a combination of drift-diffusion (DD), ensemble Monte Carlo (EMC) and kinetic Monte Carlo (KMC) simulations to study the effect of defect assisted transport (DAT) of photogenerated holes through hydrogenated amorphous silicon [a-Si:H(i)] passivation layers. We then correlate the effect of DAT on the overall device performance of SHJSC. At first the DD simulation is conducted for the entire SHJSC to determine its J-V characteristics and band profiles. We extract the valence band, hole quasi-Fermi level and electric field for the DD simulation for various device operating points (maximum power point is of particular interest). EMC is used to determine the incident carrier distribution on the barrier. Along with analytical distributions for a-Si:H [4], the KMC domain is set up to simulate the interaction of discrete carriers with discrete defects [5][6]. The KMC method uses probabilistic distributions of various physical mechanisms to ascertain the behavior of the system [7].

Our simulations indicate that multi-phonon injection is the primary process via which photogenerated holes are injected into the a-Si:H(i) passivation layer. Defect to defect (hopping) transitions is the prominent mode of transport within the a-Si:H(i) barrier. Lastly, for collection of photogenerated holes, Poole-Frenkel emission is dominant for thin a-Si:H(i) layers (< 10 nm) whereas the defect emission is dominant for thicker layer (> 10 nm).

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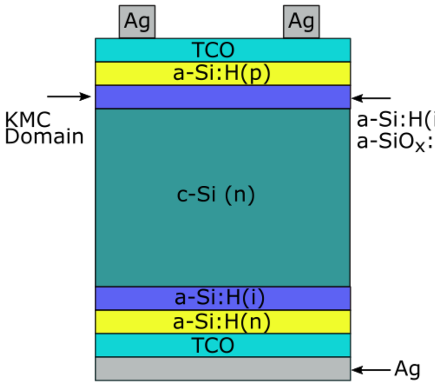

Fig.1: Schematic diagram of a silicon heterojunction solar cell. Drift-diffusion simulations are conducted for the entire cell, whereas the kinetic Monte Carlo simulation is limited to the a-Si:H(i) layer.

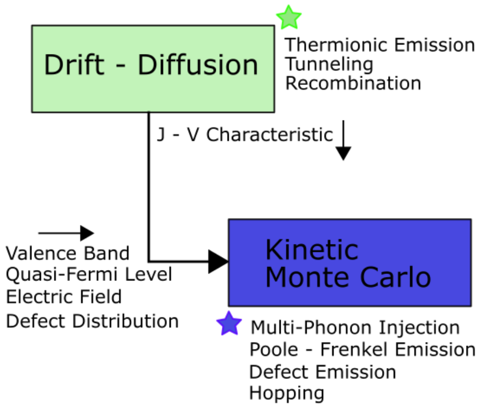

Fig.2: Flow-chart of simulation methodology.

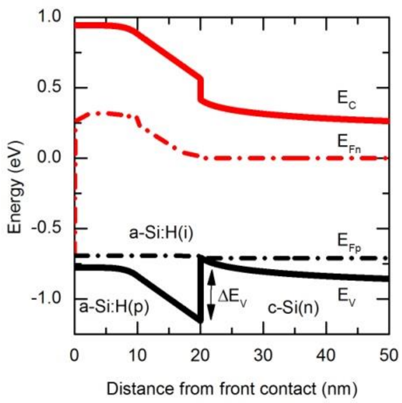

Fig.3: Energy band diagram of a SHJSC with a 10 nm thick a-Si:H(i) passivation layer at maximum power point (~ 0.693 V).

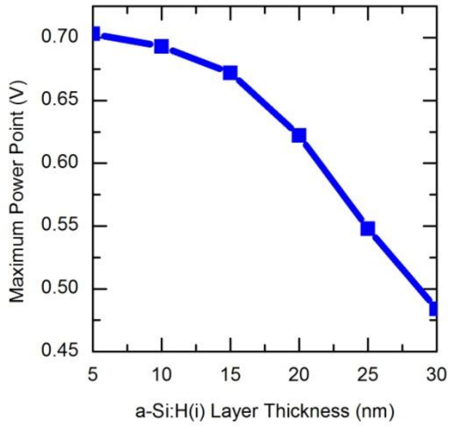

Fig.4: Maximum power point of a SHJSC vs. a-Si:H(i) thickness.

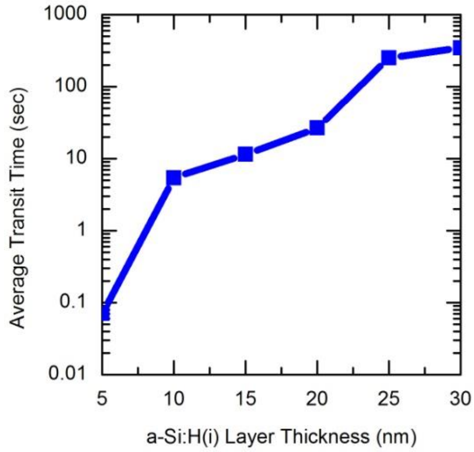

Fig.5 Average transit time (τ) for photogenerated holes to cross the a-Si:H(i) layer vs. a-Si:H(i) layer thickness at 300 K.

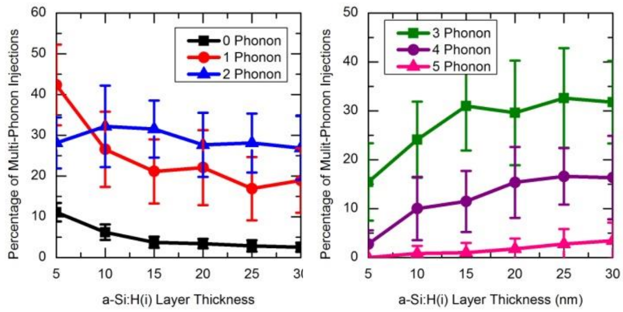

Fig.6: Percentage of phonon transitions for injection into the a-Si:H(i) barrier vs. a-Si:H(i) thickness.