A Multi-Scale Modeling Approach to Study Transport in Silicon Heterojunction Solar Cells

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INTRODUCTION

Single junction solar cells based on Silicon continue to be relevant and commercially successful in the market due to their high efficiencies and relatively low cost processing. Heterojunction solar cells based on crystalline (c-Si) and amorphous (a-Si) silicon (HIT Cells) have paved the way for devices with high V_{OC}'s (>700 mV) and high efficiencies (>20%) [1]. Last year Panasonic announced a world record efficiency of 25.6% for its trademark a-Si/c-Si HIT cell [2].

The novel structure of the device precludes the usage of traditional methods (such as drift diffusion) to accurately understand the nature of transport. Theoretical models used by commercial simulators assume a Maxwellian distribution of carriers and lack the sophistication to study defect transport. In this work we utilize a combination of Ensemble Monte Carlo (EMC) simulations to study the high field behavior of the photogenerated minority carriers at the interface and Kinetic Monte Carlo (KMC) simulations to understand defect assisted transport in the amorphous silicon layer.

THEORETICAL MODEL

In this work we simulate a HIT cell structure with a p^+ front emitter (a-Si) of 10 nm, an intrinsic buffer layer (a-Si) of 10 nm and a n type c-Si absorber layer. The potentials and fields in the device were calculated using the commercial software SILVACO at a maximum power point of 0.6 V. The goal of our work is to study the behavior of the photogenerated minority carriers in the high field region near the heterointerface and its transport through the intrinsic a-Si buffer layer via defect assisted transport.

The transport in the high field region in the c-Si region near the heterointerface is studied by implementing the EMC method. As the photogenerated carriers under consideration are holes, the EMC considers the heavy hole, light hole and split off bands to calculate hole properties. We also consider the warping and non - parabolicty of the bands which can play a significant role for hot carriers. At the a-Si/c-Si interface the EMC solver is coupled to the KMC solver. While the EMC monitors the progress of carriers in the high field region in the c-Si near the heterointerface [3], the KMC simulates defect assisted transport in the intrinsic a-Si. The EMC solver calculates the distribution function at the heterointerface and delivers it to the KMC which simulates 'hopping' of discrete carriers via point like defects till they exit the barrier via various extraction mechanisms [4].

RESULTS AND CONCLUSIONS

Fig. 1. shows the velocity vs. field characterristics for holes in warped non parabolic bands. The EMC solver shows that the carrier distribution at the heterointerface is highly non-Maxwellian (Fig. 2) due to high fields while most commercial simulators using the Drift-Diffusion method assume a Maxwellian distribution of carriers at all points within the device. The KMC solver utilizes this distribution to conduct defect assisted transport and calculates the energy distribution function (Fig. 3) and average time taken for 'hopping' transport. Fig.4 shows how the average transit time reduces with increase in the average energy of the carrier distribution at the interface. The transit time is a great indicator of how much current the device can support and the current suppression that is occurring at the heterointerface. The KMC solver results give us many valuable insights into device transport, such as the effect of phonon emission on the carrier distribution and the identification of the dominant extraction mechanism (which was Poole-Frenkel emission) for the device under consideration. We can also evaluate device characteristic for barriers with different defect densities which allows us to explore different material systems which can potentially be incorporated into a HIT cell.

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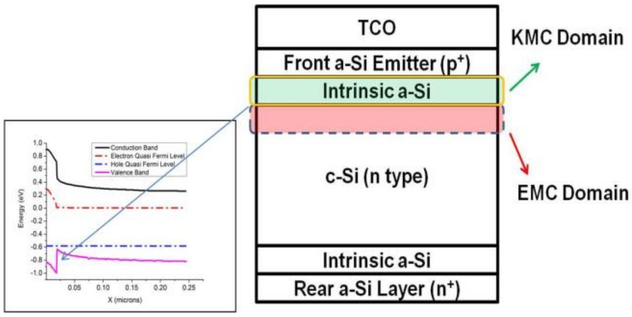

Fig. 1. Schematic diagram of a HIT cell with simulation domains. Overall electric field distribution is calculated using drift-diffusion solver coupled to a global Poisson solver (Silvaco). EMC is used to account for hot holes, which is, in turn, coupled with KMC to study in details transport through defect states in the a-Si.

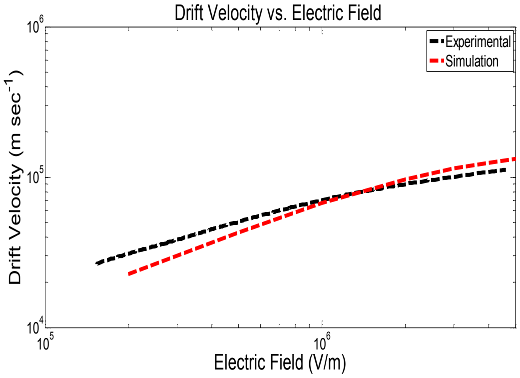

Fig. 2. Velocity vs. Electric Field for holes in c-Si.

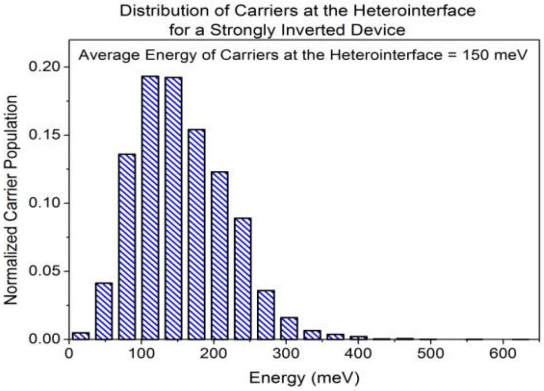

Fig. 3. Energy distribution function for a strongly inverted device at the a-Si/c-Si interface as calculated by the EMC.

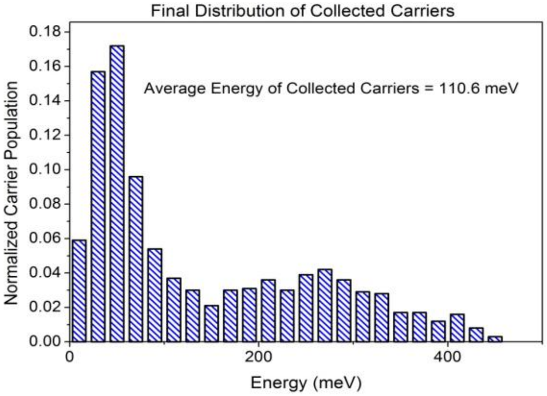

Fig. 4. The energy distribution function of the carriers after collection as calculated by the KMC.

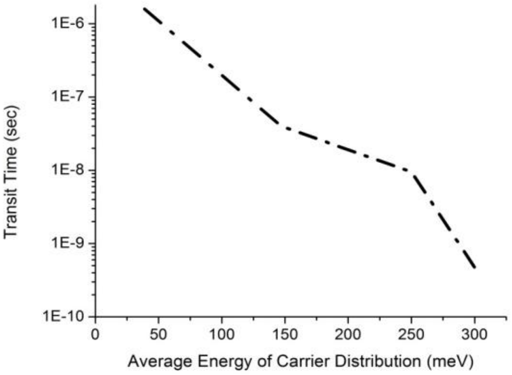

Fig. 5. Average transit time vs. average energy of carriers at the heterointerface.

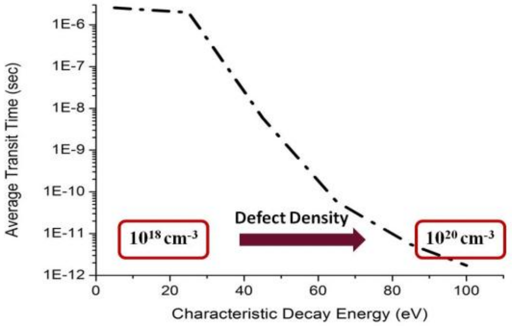

Fig. 6. Average transit time vs. characteristic decay energy (it is an indicator of the defect density present in the barrier).