Numerical simulation of metal oxide hole selective contacts for III-V/Si tandem solar cells

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The current global photovoltaic (PV) industry is dominated by single junction crystalline silicon solar cells. With the adoption of new technologies, industrial silicon solar cell efficiency will approach its fundamental limit [1] in the foreseeable future. III-V/Si multi-junction solar cells (MJSCs) are one of the most promising techniques to surpass such fundamental efficiency limit of single junction solar cells.

Epitaxial growth of III-V layers on silicon substrates is believed to be one of the most mature and stable integration approaches. Challenges associated with lattice mismatches and epitaxy of polar III-Vs on nonpolar silicon heterovalent interfaces were circumvented by employing proper silicon surface preparation and a Gallium Phosphide (GaP) nucleation layer [2], which has a small lattice mismatch to silicon (0.37% at 300 K). In addition, the relatively large bandgap of GaP (2.26 eV), together with an electron affinity (3.8 eV) close to silicon, lead to large valance band and small conduction band offsets between n-type GaP and n-type silicon. This makes GaP not only a nucleation layer for III-V epitaxial growth on silicon, but also an ideal electron selective layer for silicon solar cells.

An obvious back contact scheme for silicon in a III-V/GaP/Si tandem configuration is, therefore, employing a hole selective contact to make a GaP electron selective layer/silicon bulk absorber/hole selective layer structure. Various reported technologies can serve this purpose, e.g. Tunnel Oxide Passivated Contact (TOPCon) and heterojunction featuring amorphous silicon layers. However, due to the high thermal budget required during fabrication, TOPCon structure is less favourable. Amorphous silicon heterojunction layers are promising. But there are issues with contamination for putting III-V materials into amorphous silicon deposition chamber.

Transition metal oxides (TMOs) are attractive alternatives due to their wide range of work function and bandgap values that are important in forming carrier selective contacts for both n- and p-type crystalline silicon. In addition, thermal evaporation is often used to deposit such TMOs, which frees up the material

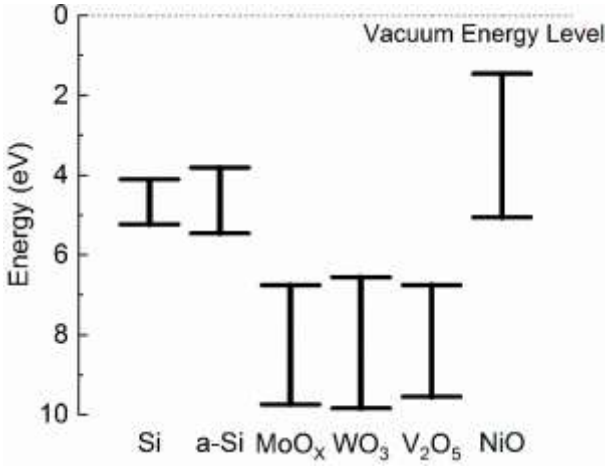

Figure 1. Bandgap and band alignment of some hole selective materials with silicon [3-6].

that can be loaded since contamination issue is less concerned in the thermal evaporator.

Many hole selective TMOs, namely Nickel oxide (NiO), Tungsten oxide (WO_3), Vanadium oxide (V_2O_5) and Molybdenum oxide (MoO_X), have been demonstrated as effective hole selective contacts for either p or n-type silicon. Figure 1 shows the bandgap and electron affinity of these hole selective materials. Two distinct hole selectivity mechanisms of these layers on silicon exist. The first one is the exceptionally large electron affinity (> 6 eV) which induces band bending in silicon that facilitates the hole extraction,

with MoO_X, WO_3 and V_2O_5 as representatives. Oxygen vacancies tend to form in these materials during the deposition and thus forming a defect band below the conduction band making them n-type. These defect levels are also important for the extraction of holes as carrier tunnelling depends on the concentration of these defects, as will be shown later. The other mechanism, represented by NiO, is via the small electron affinity and large bandgap values, which lead to high conduction and low valance band offsets with silicon. In this work, Sentaurus TCAD simulations of two representative materials, namely NiO and MoO_X, on GaP/Si/TMO structures under top $GaAs_{75}P_{25}$ junction truncated spectrum are performed. Insights into the requirements of such TMOs as hole selective layers for III-V/Si tandem cells are presented.

NiO

Depending on the deposition condition, electron affinity (thus work function) and bandgap values of TMO layers vary, which affects band alignment with silicon thus carrier selectivity is affected as well. For NiO, its electron affinity is found to be close to 1.4 eV [7]. This unusually small electron affinity together with its relatively large bandgap (ranging from ~3 to ~4.0 eV [8]) forms large conduction band and small valence band offsets when deposited on silicon, making it a hole selective material for both p and n-type silicon.

Figure 2 shows the schematic of the simulated GaP/Si/NiO cell. Front n++ doping is for contacting the unintentionally doped n-type GaP layer. Calculated band alignment between GaP, silicon and NiO layers are also shown. A large conduction band offset with a barrier height for electrons of approximately 2.7 eV is formed between NiO and silicon, effectively blocking the conduction of electrons while holes can still travel through interface freely.

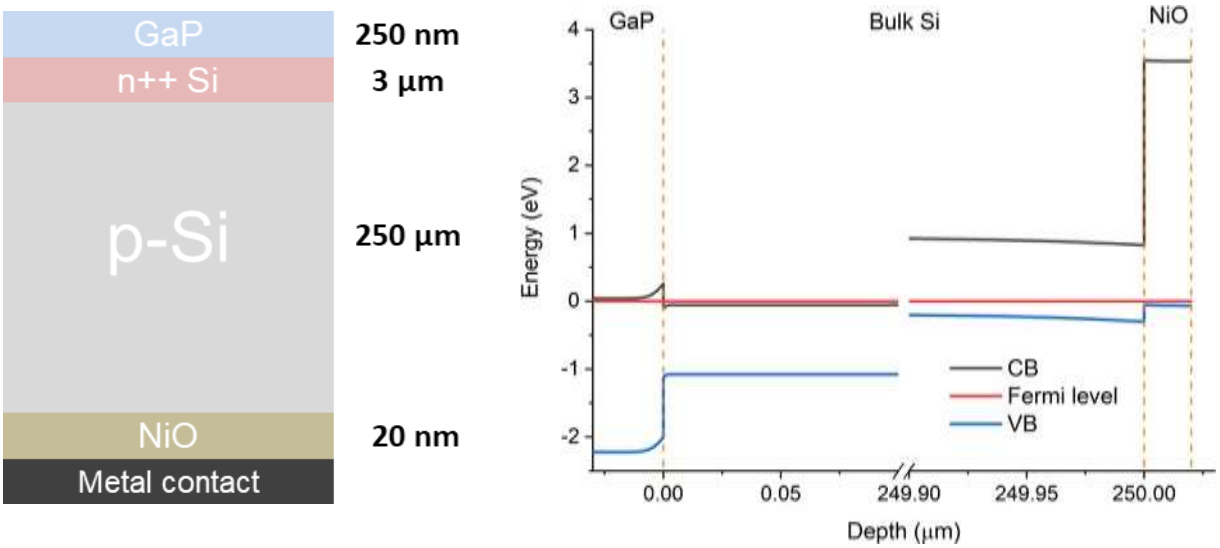

Figure 2. Left: Schematic of Sentaurus simulated GaP/Si/NiO structure. Right: Calculated band alignment of the simulated GaP/Si/NiO structure.

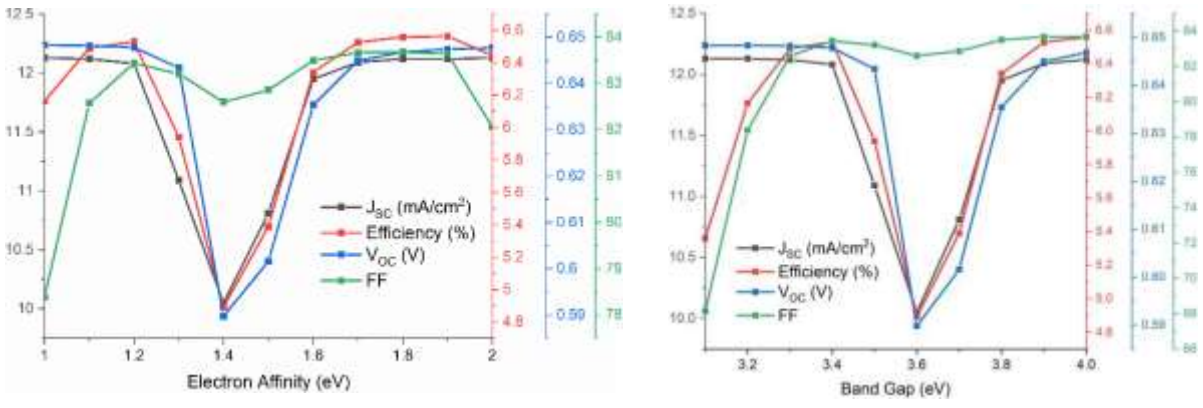

Figure 3. Simulated effect of Left: electron affinity, Right: Bandgap value of NiO on the cell performance.

Figure 3 shows the impact of different electron affinity and bandgap values of NiO on the cell performance. It can be seen that when electron affinity of the NiO is extremely small (less than 1.2 eV), barrier for the hole transport is increased due to the trend of forming an inversion layer at the interface region of silicon. This increased barrier reduces the hole conductivity and thus fill factor drops accordingly. An open-circuit voltage (V_{OC}) of 0.64 V is achievable with Si/NiO interface recombination velocity (IRV) fixed at 1000 cm/s [8], yet by employing an extra passivation layer such as intrinsic amorphous silicon layer in between silicon and NiO layer, Si/NiO IRV can be lower thus better V_{OC} value is expected.

MoO_X

In terms of MoO_X layer, its wide bandgap of ~3.6 eV and exceptionally large electron affinity of ~6.7 eV [9] induces an inversion layer at the region close to silicon surface, as shown in the calculated band alignment in Figure 3. Due to the existence of this inversion layer, valence band of the silicon is higher

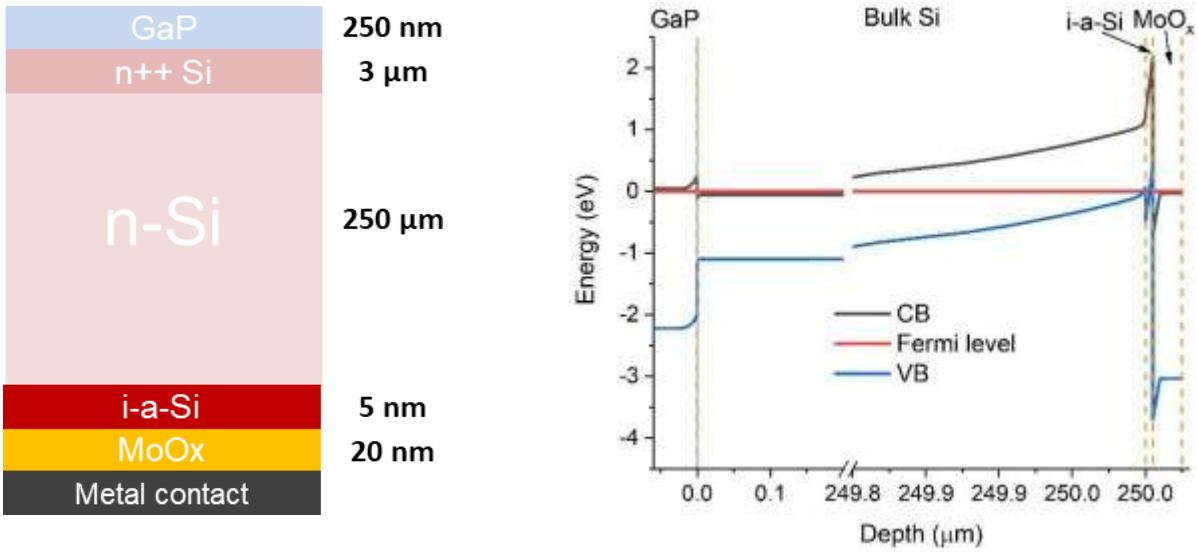

Figure 3. Left: Schematic of Sentaurus simulated GaP/Si/a-Si/MoO_X structure. Right: Calculated band alignment of the simulated GaP/Si/a-Si/MoO_X structure.

than the conduction band of the MoO_X layer, forming an extremely high barrier for hole transport, which in theory blocks all the hole extraction from silicon bulk. However, when thermal evaporation is used to deposit the MoO_X layer, the deposited layer becomes amorphous and a slightly sub-stoichiometric MoO_X forms. The reduced oxidation states in MoO_X result in high concentration of defect bands under its conduction band, allowing trap-assisted tunnelling of the holes generated in the silicon bulk. Therefore, hole selectivity becomes possible and thus greatly depends on the trap density.

In Sentaurus model for simulating the GaP/Si/a-Si/MoO_X structure, trap-assisted tunnelling is enabled in both amorphous silicon as well as the MoO_X layer. Figure 4 shows the

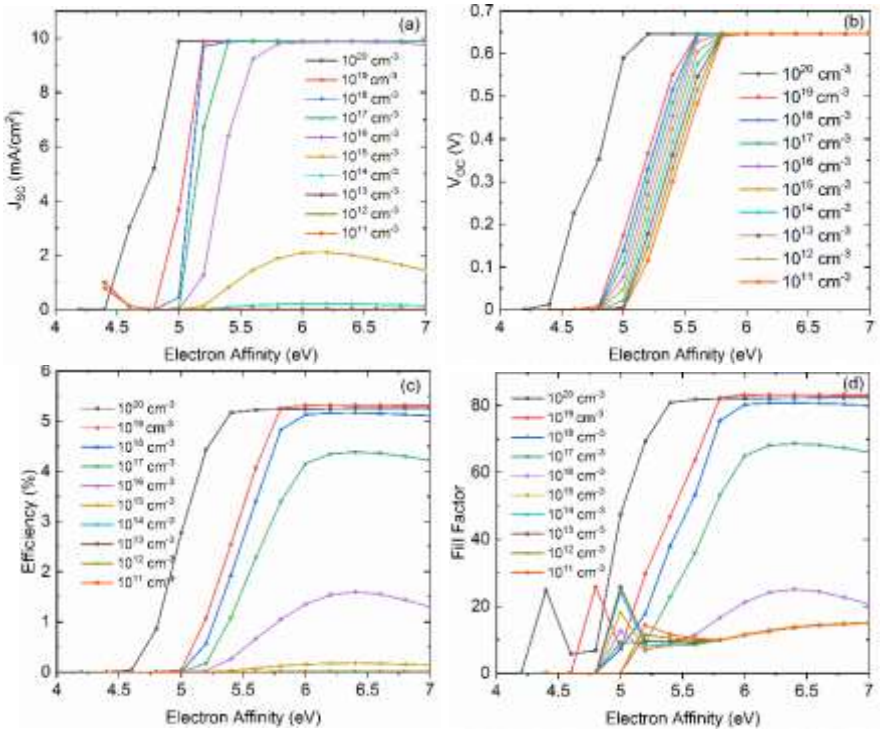

Figure 4. Effect of the trap density in MoO_X layer on the GaP/Si/a-Si/MoO_X device performance on (a) short-circuit current, (b) open-circuit voltage, (c) efficiency, (d) fill factor.

dependence of the GaP/Si/a-Si/MoO_X device performance on the trap density of the MoO_X layer. Higher trap density in MoO_X layer means larger trap-assisted tunnelling current of holes. Therefore, when the electron affinity of the MoO_X layer is the same, higher cell performance can be attained when the trap density is higher.

These results show that the cell performance critically depends on the MoO_X layer electron affinity being in the values greater than 4.5 or higher, depending on the trap densities. This highlights the importance of band alignment between the valence band of amorphous silicon and the conduction band of MoO_X layer. When the electron affinity of MoO_X layer is small, valence band of the amorphous silicon layer is lower than the conduction band of MoO_X layer, inhibiting band to band tunnelling of holes from silicon to MoO_X layer. This band to band tunnelling is more effective when the conduction band of MoO_X layer is lower than the valence band of the amorphous silicon layer. Therefore, both band to band and trap-assisted tunnelling of the holes from silicon to MoO_X layer are the key factors that enable the hole selectivity of MoO_X layer on silicon.

In conclusion, both NiO and MoO_X layers can be applied onto the rear surface of GaP/Si structure as hole selective contacts, forming a GaP electron selective/silicon bulk/TMO hole selective structure that can be integrated into III-V/Si tandem cells. Hole selectivity for NiO layer on silicon is enabled by its large bandgap value and small electron affinity, forming asymmetric band offsets for electron and holes. In terms of MoO_X layer, its hole selectivity is enabled by both trap-assisted and band to band tunnelling, which benefit from the formation of the oxide vacancies during evaporation and exceptionally large work function of the MoO_X layer.

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