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TEM studies of hole-selective molybdenum oxide contacts in silicon heterojunction solar cells

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Silicon heterojunction (SHJ) solar cells have been able to achieve very high cell efficiencies (>25 %). This was accomplished using *carrier selective contacts (CSCs)* for both the electron and hole contact regions. CSCs not only passivate the silicon surface, but also allow the flow of only one type of carrier while blocking the other. Typically, CSCs consists of an intrinsic hydrogenated amorphous silicon (a-Si:H(*i*)) passivation layer in combination with a-Si:H(*n*)/a-Si:H(*p*), which act as electron/hole-selective contacts respectively. Recently, transition metal oxides have emerged as alternative materials to be employed as either electron-selective (e.g., TiO_2) or hole-selective (e.g., MoO_x, WO_x) contacts in SHJ cells [1-3].

In the present work, the objective was to investigate the stability MoO_x-based hole-selective contacts upon low temperature anneal to be employed in SHJ cells. Sub-stochiometric MoO_x films (< 10 nm) were deposited by thermal evaporation from stochiometric MoO_3 powder on polished *n*-type {100} FZ-Si wafers after removal of the native SiO_x by hydrofluoric acid. Then, after air exposure, indium tin oxide (ITO) was deposited by reactive sputtering to act as a transparent conducting oxide (TCO) layer. For a comparative study, an a-Si:H(*i*) buffer layer was included in certain samples prior to deposition of MoO_x. Finally, some samples were annealed at 200° C for 10 min on a hot plate in ambient air.

For TEM studies, specimens were prepared by focused ion beam (FIB) milling with the help of an FEI 200 TEM FIB. Cross-sectional micrographs were obtained under bright field (BF) and high-resolution transmission electron microscopy (HRTEM) conditions with the help of an FEI Tecnai F30 TEM at an operating voltage of 300 KV.

It is evident from cross-sectional micrographs that for the samples without an a-Si:H(*i*) buffer layer, a SiO_x interlayer is formed at the c-Si/MoO_x interface, even before annealing. Moreover, the thickness of the SiO_x layer is very non-uniform. (Figure 3). The formation of SiO_x likely occurs due to a chemical reaction during the deposition of MoO_x. Furthermore, thermodynamics are favorable for the oxidation of Si by MoO_x since Mo has a higher affinity for oxygen than Si, which results in a 2-4 nm thick SiO_x interlayer which exceeds the maximum tunneling thickness (≈ 2 nm). However, SiO_x is sub-stochiometric and contains defect states, such as oxygen vacancies, which allows the conduction of charge carriers and results in a high conductivity of the SiO_x interlayer [4]. On the other hand, if an a-Si:H(*i*) buffer layer is present, then a 1-2 nm SiO_x layer is observed at a-Si:H(*i*)/MoO_x interface after annealing (Figure 2); this is consistent with observations reported by Sacchetto *et al.* [5]

Overall, the presence of the SiO_x interlayers at the c-Si/MoO_x and the a-Si:H(*i*)/MoO_x interfaces are expected to significantly impact the conduction of charge carriers through c-Si/MoO_x/ITO and c-Si/a-

Si:H(i)/MoO_x/ITO contact structures, respectively. Their band alignment and the presence of defect states within the MoO_x layer (e.g., oxygen vacancies) will be investigated in detail as part of this study.

In conclusion, TEM studies have successfully revealed oxygen diffusion across the interfaces and formation of a sub-stochiometric SiO_x interlayer at the c-Si/MoO_x and a-Si:H(i)/MoO_x interfaces. Furthermore, no interlayer was observed at the MoO_x/ITO interface, even after annealing. This work has provided valuable information about the stability of the MoO_x-based hole-selective front contacts employed in high-efficiency SHJ solar cells.

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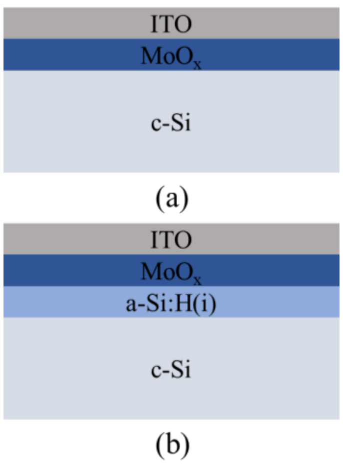

Figure 1: Schematic of test structures

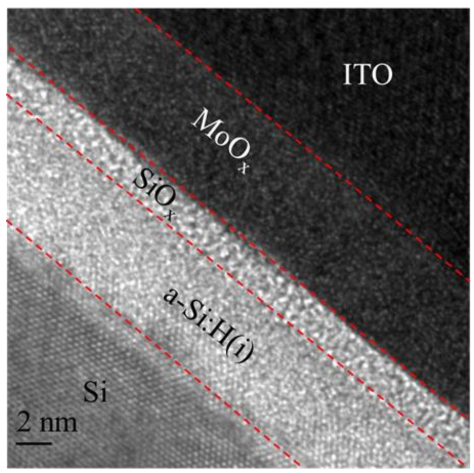

Figure 2: HRTEM image of c-Si/a-Si:H(i)/MoO_x/ITO (annealed)

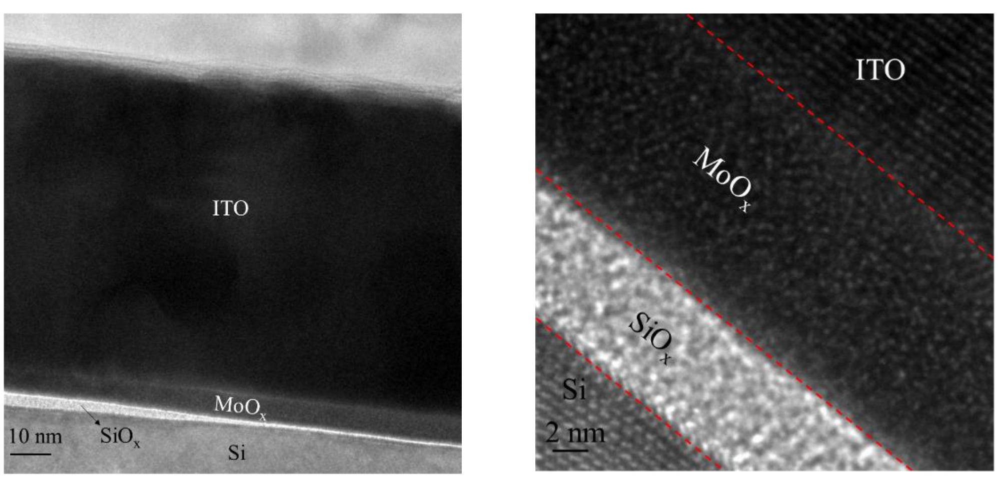

Figure 3: BF (left) and HRTEM (right) images of c-Si/MoO_x/ITO (as-deposited)

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