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

Haider Ali1,2, Geoffrey Gregory1,2, Martin Bivour3, Matthew Schneider4, Martin Hermle3, Kristopher O. Davis1,2

1. Department of Materials Science and Engineering, University of Central Florida, Orlando, FL, USA
2. Florida Solar Energy Center, University of Central Florida, Cocoa, FL, USA
3. Fraunhofer Institute for Solar Energy Systems, Heidenhofstrasse 2, D-79110 Freiburg, Germany
4. Los Alamos National Laboratory, Los Alamos, NM, USA

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., TiO2) or hole-selective (e.g., MoOx, WOx) contacts in SHJ cells [1-3].

In the present work, the objective was to investigate the stability MoOx-based hole-selective contacts upon low temperature anneal to be employed in SHJ cells. Sub-stoichiometric MoOx films (<10 nm) were deposited by thermal evaporation from stochiometric MoO3 powder on polished n-type {100} FZ-Si wafers after removal of the native SiOx 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 MoOx. 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 SiOx interlayer is formed at the c-Si/MoOx interface, even before annealing. Moreover, the thickness of the SiOx layer is very non-uniform. (Figure 3). The formation of SiOx likely occurs due to a chemical reaction during the deposition of MoOx. Furthermore, thermodynamics are favorable for the oxidation of Si by MoOx since Mo has a higher affinity for oxygen than Si, which results in a 2-4 nm thick SiOx interlayer which exceeds the maximum tunneling thickness (~2 nm). However, SiOx is sub-stoichiometric and contains defect states, such as oxygen vacancies, which allows the conduction of charge carriers and results in a high conductivity of the SiOx interlayer [4]. On the other hand, if an a-Si:H(i) buffer layer is present, then a 1-2 nm SiOx layer is observed at a-Si:H(i)/MoOx interface after annealing (Figure 2); this is consistent with observations reported by Sacchetto et al. [5].

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

References

Figure 1: Schematic of test structures

![Figure 1](https://doi.org/10.1017/S1431927618008024)

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

![Figure 2](https://doi.org/10.1017/S1431927618008024)

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