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TEM Study of MoO_x/Ni and MoO_x/Al Contacts for Silicon Solar Cells

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Carrier-selective contacts are used at both the front and rear contact regions of silicon solar cells to increase solar cell efficiency. These carrier-selective contacts allow the flow of only one type of carrier while blocking the other, and when combined with thin surface passivation layers, they can drastically lower carrier recombination losses. More recently, it has been demonstrated that both electron-selective and hole-selective contacts can be formed using transition metals oxides. Often, a transition metal oxide is sandwiched between a metal contact (e.g., Al) and a suitable passivation layer (e.g., a-Si:H(i), SiO_2). For instance, Yang *et al.* reported solar cell efficiencies up to 21.6% using SiO_2/TiO_2/Al as an electron-selective rear contact. [1, 2]. Likewise, MoO_x has been demonstrated to be an effective hole-selective contact due to its wide band gap (≈ 3 eV) and high work function (≈ 6.6 eV).[3, 4]

In the present work, the objective was to investigate low temperature stability of contact structures formed by combination of MoO_x with Ni and Al metal to be employed as hole-selective contacts in crystalline silicon (c-Si) solar cells. Planar 200 µm thick 1 Ω-cm *p*-type c-Si wafers were used in this study. At first, the wafers were subjected to HF clean to remove the native oxide layer followed by exposure to UV-ozone treatment for 10 minutes to form a self-limiting SiO_x layer (<1.5 nm) on the Si surface. Subsequently, a thin (< 5 nm) MoO_x was deposited was Si substrate by atomic layer deposition (ALD). Finally, Ni and Al contacts were formed over MoO_x by evaporation under identical e-beam conditions. Select test structures were then annealed in air at 200°C.

Cross-sectional TEM specimens were prepared by focused ion beam (FIB) milling technique with the help of FEI 200 TEM FIB. TEM studies were performed with the help of FEI Tecnai F30 TEM at an operating voltage of 300 KV.

Cross-sectional high-resolution TEM (HRTEM) images obtained for various samples are shown in Figure 1. It can be seen in Figures 1(a) and 1(b) that no significant change occurs due to HF treatment in case of c-Si/SiO_x/MoO_x/Ni/Al contact. Moreover, no NiO_x interlayer was observed at MoO_x/Ni interface even after annealing at 200°C (Figure 1(c)). Likewise, no apparent interlayer is observed at MoO_x/Al interface even after annealing in case of c-Si/SiO_x/MoO_x/Al contact (Figure 1(d)). It is quite possible that some oxygen diffusion may have occurred across MoO_x/Al interface into the Al layer due to higher oxygen affinity of Al compared to Mo. However, the oxygen diffusion was not enough to result in the formation of a distinct AlO_x interlayer at the MoO_x/Al interface.

In summary, HRTEM images revealed that no interlayer formation occurs at MoO_x/Al as well as MoO_x/Ni interfaces even after annealing at 200°C. Overall, it is evident that no significant elemental diffusion occurred across interfaces in case of both c-Si/SiO_x/MoO_x/Ni/Al and c-Si/SiO_x/MoO_x/Al contact structures.

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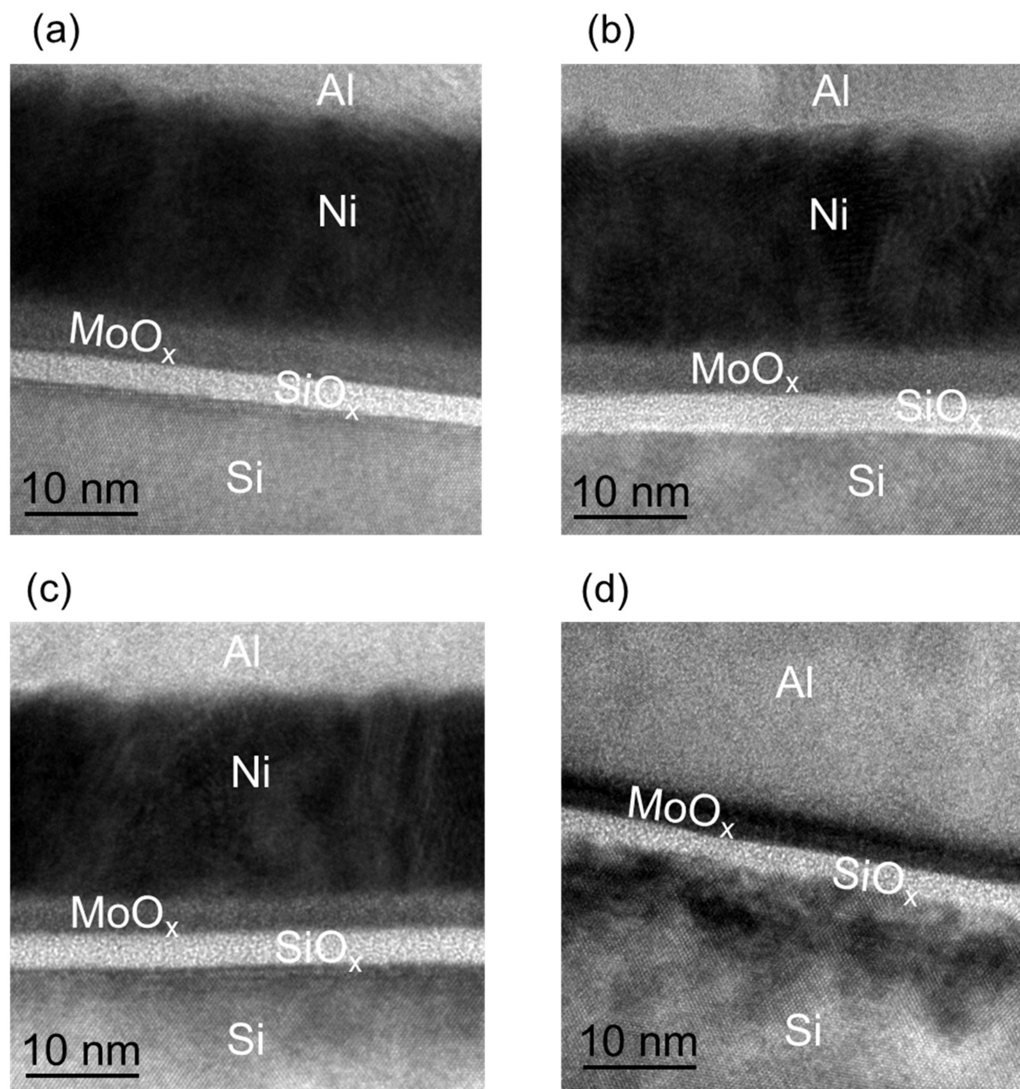

Figure 1. Cross-sectional HRTEM images of c-Si/SiO_x/MoO_x/Ni/Al contact (a) no HF, no anneal; (b) HF clean, no anneal; (c) HF clean, annealed @200°C; (d) c-Si/SiO_x/MoO_x/Al contact annealed @ 200°C

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