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TEM studies of TiO_2-based passivated contacts in c-Si solar cells

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In order to achieve ultra-high efficiency for crystalline silicon (c-Si) solar cells, it is essential to have very low recombination velocities at both contact and non-contact areas. One of the techniques employed for this purpose is the so-called *passivated contact*, which is realized by depositing an ultra-thin oxide film which can not only passivate the silicon surface, but also allow only one type of carrier, i.e. either electron or hole to pass through it. Some of these oxides which have been employed as passivated contacts in c-Si solar cells include SiO_2, Al_2O_3, TiO_2 and MoO_x.[1-5]

In the present work, the objective was to investigate TiO_2-based passivated contacts for c-Si solar cells. Ultra-thin TiO_2 films (<5 nm) were deposited by ALD on (100) n-type Si wafers. Some samples were subject to thermal oxidation prior to TiO_2 deposition to allow an ultra-thin SiO_2 (<2 nm) layer to grow. For comparative studies, in some samples Al contacts (≈2-3 µm) were formed over TiO_2 layer by evaporation. The samples were then studied under transmission electron microscope (TEM) prior to as well as after forming gas anneal (FGA).

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 F 30 TEM under operating voltage of 300 KV. Cross-sectional micrographs of contacts were obtained under bright field (BF) and high resolution transmission electron microscopy (HRTEM) conditions with a point-to-point resolution was 0.2 nm. Compositional analysis was carried out with the help of electron energy loss spectroscopy (EELS) technique, since EELS is well suited for low atomic number elements. Gatan image filter model 200 (GIF 200) spectrometer was used for this purpose. Elemental maps were obtained by energy-filtered transmission electron microscopy (EFTEM).

Figure 1 shows the cross-sectional micrographs of as-deposited sample wherein Al contacts are formed over ultra-thin TiO_2 film which was deposited on silicon wafer by ALD. O and Ti elemental maps for the sample are shown in Figure 2.

From the cross-sectional micrographs, it can be seen that an intermediate layer is formed at Al/TiO_2 interface. Similarly, one can observe that an ultra-thin native oxide is formed at the silicon surface. It is also revealed that Al contacts formed over TiO_2 are polycrystalline. On the other hand, no crystallization of TiO_2 was observed even after annealing. Likewise, no remarkable interface change occurred after annealing and no contacts were formed between Al and Si through ultra-thin TiO_2.

From the EFTEM elemental maps, information about chemical changes occurring at the interfaces were obtained. At the Al/TiO_2 interface, Al is oxidized and an intermediate layer is formed which has no observable presence of Ti. Moreover, it can be clearly seen that TiO_2 layer is reduced to a highly oxygen deficient TiO_{2-x}. This can be explained by the fact that Al lies below Ti in the Ellingham diagram.

In conclusion, TEM studies have successfully revealed oxygen diffusion across the interfaces and formation of an intermediate layer at Al/TiO_2 interface. This work has provided us valuable information about stability of TiO_2-based passivated contacts which can be immensely useful for understanding their passivation behavior.

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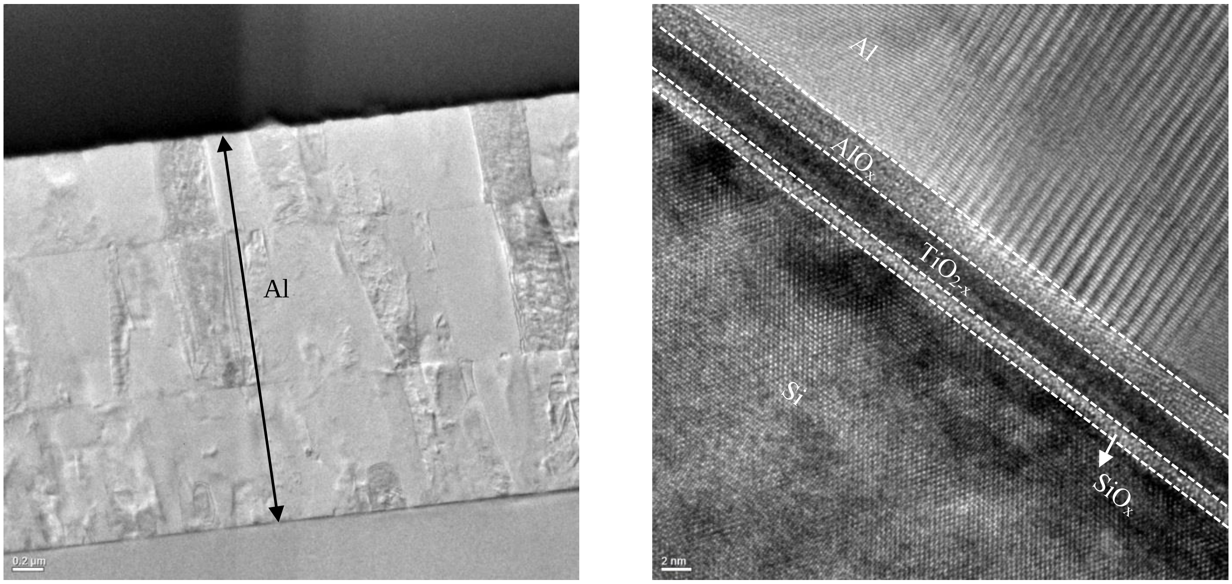
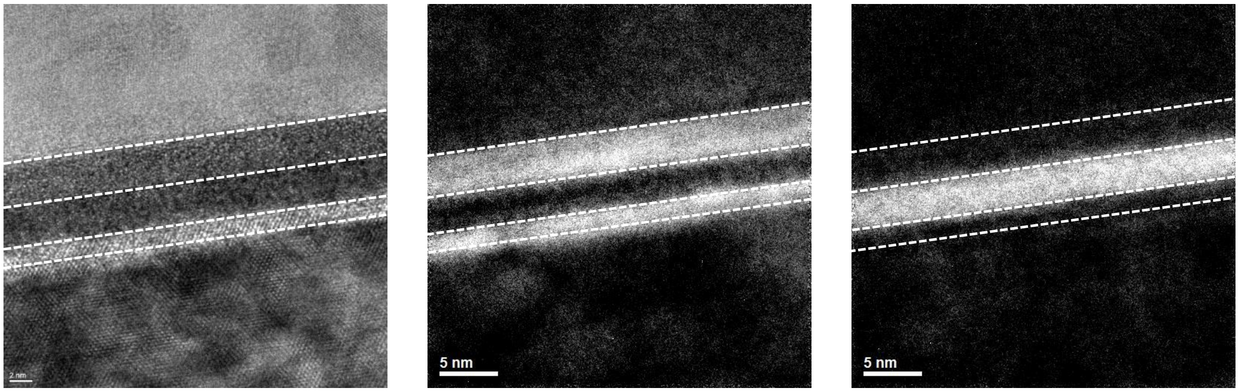


(a) Al contact (b) TiO_2 deposited on silicon by ALD

Figure 1: cross-sectional TEM micrographs of as-deposited sample



(a)HRTEM image (b) Oxygen map (c) Titanium map

Figure 2: EFTEM elemental maps for Oxygen and Titanium